Stochastic optimal control formalism for an open quantum system

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A stochastic procedure is developed which allows one to express Pontryagin's maximum principle for a dissipative quantum system solely in terms of stochastic wave functions. Time-optimal controls can be efficiently computed without computing the density matrix. Specifically, the proper dynamical update rules are presented for the stochastic costate variables introduced by Pontryagin's maximum principle, and restrictions on the form of the terminal cost function are discussed. The proposed procedure is confirmed by comparing the results to those obtained from optimal control on Lindbladian dynamics. Numerically, the proposed formalism becomes time and memory efficient for large systems, and it can be generalized to describe non-Markovian dynamics.

I. INTRODUCTION

Modern quantum technology [1], including quantum computation [2–10], quantum sensing, metrology, and imaging [11–20], and quantum communication [21–27], commonly relies on coherent control of the state of the system. A typical quantum task starts from an easily prepared initial state, undergoes a designed control protocol, and hopefully ends up with a state sufficiently close to the target state (not necessarily known in advance). When the closeness to the target state can be characterized by a scalar "terminal cost function," this quantum problem can be mathematically formulated as an optimal control problem. Many quantum applications (or at least an intermediate step of the application) fit this description. Relevant examples include state preparation [28–31], where the cost function is the overlap with the known target state; "continuous-time" variation-principle-based quantum computation [7,9,32–34], where the cost function is the ground-state energy; and quantum parameter estimation [20,35], where the cost function is the quantum Fisher information.

Pontryagin's maximum principle (PMP) [36–39] is a powerful formalism in classical control theory, and it has been applied to quantum state preparation [28,40] and nonadiabatic quantum computation [41,42]. Due to the linearity of Schrödinger's equation, PMP implies the time-optimal control typically has the so-called *bang-bang* form (the control takes its extreme values); the bang-bang form puts strong constraints on the structure of optimal solutions and is found to be the case in some problems [28,41,43]. For general quantum problems, however, the optimal control often includes a singular part [40,42,44,45], which makes PMP less informative about the solution. While one can, in principle, explicitly solve for the behavior on the singular arcs [40], such analysis is restricted to small systems as it quickly becomes intractable.

The main usefulness of PMP thus appears to be numerical: first, it provides an efficient way to compute the gradient of the terminal cost function; second, PMP gives the necessary conditions for an optimal solution which can be used to check the quality of any numerical solutions.

The application of PMP to quantum dissipative systems using a Lindblad master-equation approach has been proposed and discussed in the literature [46–49]. In Ref. [40] we demonstrated that the singular controls are essential in open systems by examining the PMP optimality conditions. In this paper, we develop a stochastic formalism to evaluate important quantities introduced by PMP. Specifically, we derive a procedure to consistently update the wave function and its costate for the stochastic Schrödinger equation so that the optimal control can be determined without constructing the density matrices. The procedure is checked against the results obtained using the Lindbladian equation. The proposed stochastic procedure not only saves time and memory for simulating large systems but can be helpful for problems in which the wave function description is intuitive, such as gate-based quantum computation [4–6,50–53], quantum error correction [54–57], and coherent feedback control [58]. Moreover, the generalization to describe systems coupled to a non-Markovian bath [59–61] is straightforward.

The rest of the paper is organized as follows. In Sec. II we recapitulate relevant conclusions from classical control theory. In particular, we express important quantities introduced by PMP in terms of the density matrix which are essential for open quantum systems. In Sec. III we describe how to use the stochastic Schrödinger equation to simulate the dissipative system, with an emphasis on determining the optimal control. In Sec. IV we numerically implement the proposed stochastic procedure to the single-qubit system. In particular we compare the results from the deterministic Lindbladian with those from the stochastic Schrödinger equation. A brief conclusion is given in Sec. V.

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II. DENSITY-MATRIX FORMULATION AND PONTRYAGIN'S MAXIMUM PRINCIPLE

Consider a quantum system characterized by the density matrix ρ, evolving in time under some general Markovian quantum dynamics

$$\dot{\rho} = \mathcal{L}_t[\rho], \tag{1}$$

with $\mathcal{L}_t$ being a Liouvillian superoperator which depends on some control variable $u(t)$. In particular, we will be concerned with dynamical systems with linear controls such that $\mathcal{L}_t = \mathcal{L}_0 + u(t)\mathcal{L}_u$, where $\mathcal{L}_0$ represents the bare dynamics of the system beyond our control and $\mathcal{L}_u$ is the controllable part. The control field $u(t)$ is further assumed to be bounded $|u(t)| \leqslant 1$. While most of our discussion is completely general and applies to arbitrary Liouvillians, we are primarily concerned with coherent controls, i.e.,

$$\mathcal{L}_u[\rho] = -i[H_u, \rho], \tag{2}$$

where H_u is the part of the Hamiltonian that can be controlled. Moreover, the present goal is to maximize the overlap between the final state at time t_f and the target state $|\psi_{\text{tar}}\rangle$, which can be expressed by the terminal cost function $\mathcal{C}$ (to minimize),

$$\mathcal{C}(t_f) = -\text{Tr}[\rho(t_f)\rho_{\text{tar}}] = -\langle\psi_{\text{tar}}|\rho(t_f)|\psi_{\text{tar}}\rangle. \tag{3}$$

This cost function has the benefit of being linear in the state $\rho(t_f)$. Notice that for a pure target state $\langle\psi_{\text{tar}}|\rho(t_f)|\psi_{\text{tar}}\rangle$ corresponds to the standard Uhlmann fidelity [62,63]. Here we shall focus the discussion on a target state that is pure, but since the cost function is just the Hilbert-Schmidt inner product between the terminal state and the target state, the same cost function could be used for mixed states as well. Following PMP, we proceed by introducing the control Hamiltonian (c-Hamiltonian) $\mathcal{H}_c$,

$$\mathcal{H}_c = \text{Tr}(\lambda\dot{\rho}) = (\lambda\mathcal{L}_0[\rho]) + u(t)\text{Tr}(\lambda\mathcal{L}_u[\rho]), \tag{4}$$

which is a *real-valued* scalar and should not be confused with the Hamiltonian H of the system [64]. The c-Hamiltonian $\mathcal{H}_c$ is constructed such that one of Hamilton's equations simply yields the equation of motion for the state, i.e.,

$$\dot{\rho} = \frac{\partial\mathcal{H}_c}{\partial\lambda}, \tag{5}$$

where the canonical momentum λ, typically referred to as the costate in the context of optimal control, satisfies

$$\dot{\lambda} = -\frac{\partial\mathcal{H}_c}{\partial\rho}. \tag{6}$$

The initial condition for the state is typically $\rho(t_0) = \rho$, and according to PMP, the boundary condition for the costate should satisfy

$$\lambda(t_f) = \frac{\partial\mathcal{C}(t_f)}{\partial\rho(t_f)} = -|\psi_{\text{tar}}\rangle\langle\psi_{\text{tar}}|. \tag{7}$$

Necessary conditions for optimal solutions to the time-optimal control problem are simultaneously satisfying Eqs. (5) and (6), together with $\mathcal{H}_c = \text{const}$ over the entire

interval t_0 to t_f and

$$u(t) = \begin{cases} +1 & \text{if } \Phi(t) < 0, \\ -1 & \text{if } \Phi(t) > 0, \\ \text{undetermined} & \text{if } \Phi(t) = 0, \end{cases} \tag{8}$$

with the switching function $\Phi(t) = \text{Re}(\text{Tr}[\lambda\mathcal{L}_u[\rho]])$, which for coherent controls becomes

$$\Phi(t) = \text{Im}\{(\text{Tr}(\lambda[H_u, \rho])\}. \tag{9}$$

It is worth noting that the switching function corresponds to the gradient of the terminal cost function, i.e., $\Phi(t) \sim \frac{\partial\mathcal{C}}{\partial u(t)}$. When the goal is to minimize $\mathcal{C}$, $u(t)$ takes the extreme value with a sign opposite to $\Phi(t) \neq 0$; this is referred to as "bang control" and is exactly Eq. (8). When $\Phi(t) = 0$ for a finite amount of time, the controls might not be extremal, and their structure can be determined by looking at higher time derivatives of the switching function. This is beyond the present discussion, but some complementary derivations, including a discussion of singular controls, can be found in Refs. [40,42].

Before moving on to discuss stochastic dynamics, let us consider some particularly relevant dynamics. First of all, consider the dynamics to be unitary such that $\mathcal{L}[\rho] = -i[H, \rho]$. The c-Hamiltonian then reads

$$\mathcal{H}_c = \text{Im}\{\text{Tr}(\lambda[H, \rho])\} = -\text{Im}\{\text{Tr}(\rho[H, \lambda])\}, \tag{10}$$

where the latter just follows from the cyclic properties of the trace. Consequently, the costate evolution,

$$\dot{\lambda} = -i[H, \lambda], \tag{11}$$

is identical to that of the state ρ. This is not the case for dissipative dynamics; consider, for example,

$$\mathcal{L}[\rho] = L\rho L^\dagger - \frac{1}{2}(L^\dagger L\rho + \rho L^\dagger L), \tag{12}$$

where L are Lindblad jump operators. The c-Hamiltonian now takes the form

$$\mathcal{H}_c = \text{Re}\big(\text{Tr}\big[\lambda\big\{L\rho L^\dagger - \tfrac{1}{2}(L^\dagger L\rho + \rho L^\dagger L)\big\}\big]\big)$$
$$= \text{Re}\big(\text{Tr}\big[\rho\big\{L^\dagger\lambda L - \tfrac{1}{2}(L^\dagger L\lambda + \lambda L^\dagger L)\big\}\big]\big); \tag{13}$$

consequently, the costate evolution

$$\dot{\lambda} = -\big[L^\dagger\lambda L - \tfrac{1}{2}\{L^\dagger L, \lambda\}\big], \tag{14}$$

where the anticommutator is defined as $\{A, B\} = AB + BA$. Note that in the case of Hermitian jump operators Eq. (14) simply amounts to a time reversal $t \to -t$ of Eq. (12). The sum of Eqs. (10) and (13) gives the c-Hamiltonian for systems with both unitary and dissipative dynamics. In principle, optimal control solutions can be found by iteratively solving for the (co)state, extracting the switching function, and updating the controls [40]. The downside is that one has to explicitly propagate the density matrix and its costates.

III. STOCHASTIC CONTROL

In this section we describe the proposed stochastic procedure that extracts the switching function and related quantities from a stochastic Schrödinger simulation by properly correlating the Poisson random processes between the wave function and its costate. The limitation of the procedure will also be pointed out.

A. Stochastic simulation of density matrix

The formalism to simulate the density matrix ρ [Eq. (12)] by averaging the stochastic wave function was developed in the early days of quantum optics [65–67]. To facilitate later discussion, we briefly review it. Denoting $|d\psi\rangle \equiv |\psi(t + dt)\rangle - |\psi(t)\rangle$, the stochastic update of the wave function is given by

$$|d\psi\rangle = G|\psi\rangle dt + (L|\psi\rangle - |\psi\rangle)dN(t), \quad (15a)$$

where

$$G|\psi\rangle = \left[-iH - \frac{\gamma}{2} L^\dagger L + \frac{\gamma}{2} \mathbb{1}\right]|\psi\rangle. \quad (15b)$$

In Eqs. (15), $dN(t)$ is the Poisson random variable whose mean and variance are both γdt, i.e., $dN(t) = dN(t)^2 = \gamma dt$; H is the Hamiltonian of the system. The wave function evolves forward in time as $|\psi(t)\rangle \rightarrow |\psi(t + dt)\rangle = |\psi(t)\rangle + |d\psi(t)\rangle$. The density matrix can then simply be extracted as $\rho = \mathbb{E}[|\psi(t)\rangle\langle\psi(t)|]$, with the expectation value taken over the Poisson process (with the same initial state $|\psi_{\text{ini}}\rangle$) that generates the quantum jumps:

$$\rho(t) = \mathbb{E}[|\psi(t)\rangle\langle\psi(t)|] \approx \frac{1}{N} \sum_{n=1}^{N} |\psi^{(n)}(t)\rangle\langle\psi^{(n)}(t)|, \quad (16)$$

where the superscript n labels the nth realization. The same procedure can be repeated for the costate λ by unraveling it in stochastic wave function $|\pi\rangle$. Recall that the costate needs to evolve backward in time from t_f; hence, denoting $|-d\pi\rangle \equiv |\pi(t - dt)\rangle - |\pi(t)\rangle$, one has

$$|-d\pi\rangle = \tilde{G}|\pi\rangle dt + (L^\dagger|\pi\rangle - |\pi\rangle)dN(t), \quad (17a)$$

$$\tilde{G}|\pi\rangle = \left[iH - \frac{\gamma}{2} L^\dagger L + \frac{\gamma}{2} \mathbb{1}\right]|\pi\rangle. \quad (17b)$$

$dN(t)$ is again the Poisson random variable with mean and variance of γdt; further note that $\tilde{G} = G^\dagger$. To extract λ, one repeats Eq. (17) to obtain $|\pi^{(n)}\rangle$ starting from the same final state $|\pi(t_f)\rangle$, the costate density matrix is then computed using

$$\lambda(t) = \mathbb{E}[|\pi(t)\rangle\langle\pi(t)|] \approx \frac{1}{N} \sum_{n=1}^{N} |\pi^{(n)}(t)\rangle\langle\pi^{(n)}(t)|. \quad (18)$$

It is worth noting that the stochastic procedure outlined in Eqs. (16) and (18) does *not* apply to cases of negative γ even though the Lindbladian equation can be solved no matter what the sign of γ is. Since the stochastic procedure always increases the entropy, it can describe only the forward propagation of ρ and backward propagation of λ. We also point out that both Eqs. (16) and (18) can be used to simulate the mixed state. One simply has to, in conjunction with sampling the Poisson process, take random samples out of the initial density matrix.

B. Two stochastic procedures for the switching function

For the specific cost function given by expression (3), the boundary condition for the costate becomes $\lambda(t_f) = -|\psi_{\text{tar}}\rangle\langle\psi_{\text{tar}}|$. The switching function $\Phi(t)$ can thus straightforwardly be computed from Eq. (9) with $\rho(t)$ from Eq. (16) and $\lambda(t)$ from Eq. (18). Once $\rho(t)$ and $\lambda(t)$ are known, the

c-Hamiltonian can also be evaluated using Eqs. (10) and (13). This procedure works generally, and a numerical example will be provided in Sec. IV B. In this procedure, ρ and λ have to be constructed explicitly, which makes the procedure numerically quite involved; for example, one has to store all stochastic realizations of $|\psi^{(n)}(t)\rangle$ and $|\lambda^{(n)}(t)\rangle$ and then explicitly perform the trace in (9).

In the first procedure just described, the Poisson random variables that generate the state and the costate are completely uncorrelated. By correlating the random variables, however, the switching function can be obtained without computing ρ and λ explicitly as long as the terminal cost function is a linear function of the state ρ. This is natural in many situations, and the present cost function (3) is clearly of that form.

To see how the second procedure works, consider first the cost function (3). Expressed in terms of stochastic wave functions $|\psi\rangle$, this becomes

$$\mathcal{C}(t_f) = -\langle\psi_{\text{tar}}|\mathbb{E}[|\psi\rangle\langle\psi|]|\psi_{\text{tar}}\rangle = -\mathbb{E}[|\langle\psi_{\text{tar}}|\psi\rangle|^2]. \quad (19)$$

The linearity ensures that we can interchange the order in which we take the quantum expectation value and the average of the classical random process. Hence, consider the nth stochastic realization defined by the Poisson random process $dN^{(n)}(t)$, $|\psi^{(n)}\rangle$, and its costate $|\pi^{(n)}\rangle$, where the latter satisfy Eqs. (15a) and (17a) [with the same $dN(t)$], respectively; then

$$\mathcal{C}(t_f) \approx -\frac{1}{N} \sum_{n} |\langle\psi_{\text{tar}}|\psi^{(n)}(t_f)\rangle|^2 \equiv -\frac{1}{N} \sum_{n} \mathcal{C}^{(n)}(t_f). \quad (20)$$

Consequently, according the PMP, the boundary condition for the nth realization of the costate $|\pi^{(n)}(t)\rangle$ is fixed by

$$|\pi^{(n)}(t_f)\rangle = \frac{\partial \mathcal{C}^{(n)}(t_f)}{\langle\psi^{(n)}(t_f)|} = -|\psi_{\text{tar}}\rangle\langle\psi_{\text{tar}}|\psi^{(n)}(t_f)\rangle. \quad (21)$$

The switching function is then computed as

$$\Phi(t) = \frac{1}{N} \sum_{n=1}^{N} \Phi^{(n)}(t), \quad \Phi^{(n)}(t) = \text{Im}\langle\pi^{(n)}(t)|H_u|\psi^{(n)}(t)\rangle. \quad (22)$$

In contrast to the naive (first) procedure, the latter does not explicitly estimate any density matrix, which saves time and computer memory. Note that, apart from the Poisson random processes used in $|\psi\rangle$ and $|\pi\rangle$ being identical in every realization, the nth costate also explicitly depends on the nth solution of state $|\psi\rangle$ through its boundary condition.

Equation (22) can be generalized to compute other quantities. In particular, $\text{Im}\{\text{Tr}(\lambda[H, \rho])\}$ in Eq. (10) can be evaluated by replacing H_u by $H(t)$ in Eq. (22); the anticommutator $\text{Re}(\text{Tr}\lambda\{L^\dagger L, \rho\})$ in Eq. (13) can be evaluated by averaging over $\text{Re}[\langle\pi^{(n)}(t)|L^\dagger L|\psi^{(n)}(t)\rangle]$. These expressions are numerically tested (not shown). The c-Hamiltonian $\mathcal{H}_c$, however, can be computed using only the first stochastic procedure because $\text{Tr}(\lambda L\rho L^\dagger)$ cannot be expressed as the average of stochastic realizations in the form of Eq. (22).

To conclude this section, we notice that Eq. (15) is by no means the unique stochastic unraveling. Notably, when $L = L^\dagger$, one can define $H - i\gamma(t)L$ as the non-Hermitian Hamiltonian where $\gamma(t)$ is the Gaussian random process with dt-dependent variance; averaging many stochastic realizations also properly simulates the Lindblad equation

[66,67]. Both proposed procedures for the switching function, particularly the second one that correlates the random variables for $|\psi\rangle$ and $|\pi\rangle$, apply to this stochastic implementation as well (tested, not shown). An interesting open question is to consider the non-Markovian random process, beyond the Lindbladian formalism.

IV. NUMERICAL IMPLEMENTATION

In this section we confirm the proposed formalism by applying it to the specific single-qubit problem where the numerically exact solutions are nontrivial but known.

A. Single-qubit problem

To numerically test the proposed formalism, we consider a dissipative qubit system where the density matrix satisfies the Lindbladian equation:

$$\frac{\partial}{\partial t}\rho = -i[H(t), \rho] + \gamma\left[L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}\right]. \quad (23)$$

For unitary dynamics, we consider the Landau-Zener-type Hamiltonian where $H(t) = H_0 + u(t)H_u = \sigma_x + u(t)\sigma_z$, with $u(t)$ being the single control field bounded by $|u(t)| \leqslant 1$ and σ's denoting Pauli matrices [44,45]. For dissipative dynamics, we choose $L = \sigma_x$, $\gamma = 0.5$, and a total evolution time of $t_f = 0.9\pi$. These parameters produce nontrivial control protocols [40]; in particular, the combined choice of H and L leads to an optimal control that prevents the system from decaying to the maximal-entropy state even when $t_f \to \infty$, independent of the initial and target states.

Two sets of initial and target states are considered: the state-retention problem where the initial and target states $|\psi_{\text{ini}}\rangle$ and $|\psi_{\text{tar}}\rangle$ are

$$|\psi_{\text{ini}}\rangle = |\psi_{\text{tar}}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (24)$$

and the state-preparation problem where

$$|\psi_{\text{ini}}\rangle = \frac{1}{\sqrt{10 + 4\sqrt{5}}}\begin{bmatrix} 1 \\ -2 - \sqrt{5} \end{bmatrix},$$

$$|\psi_{\text{tar}}\rangle = \frac{1}{\sqrt{10 - 4\sqrt{5}}}\begin{bmatrix} 1 \\ 2 - \sqrt{5} \end{bmatrix}. \quad (25)$$

The corresponding density matrix is given by $\rho = |\psi\rangle\langle\psi|$: for the state-retention problem, $\rho_{\text{ini}} = \rho_{\text{tar}} = \frac{1}{2}(\mathbb{I} + \sigma_x)$; for the preparation, $\rho_{\text{ini (tar)}} = \frac{1}{2}[\mathbb{I} - \frac{1}{\sqrt{5}}\sigma_x - (+)\frac{2}{\sqrt{5}}\sigma_z]$. The boundary condition of the costate is given by $\lambda(t_f) = -|\psi_{\text{tar}}\rangle\langle\psi_{\text{tar}}|$. The choices of Eqs. (24) and (25) describe two limits: the initial and target states are close to (identical here) or far away from each other. Using the formalism developed in Ref. [40], the optimal controls, switching functions, and c-Hamiltonians for both problems are given in Fig. 1; these solutions are referred to as the "exact" solutions and will serve as the reference for comparison.

B. Switching functions

We now compute the switching functions using both procedures outlined in Sec. III B. The first procedure requires the
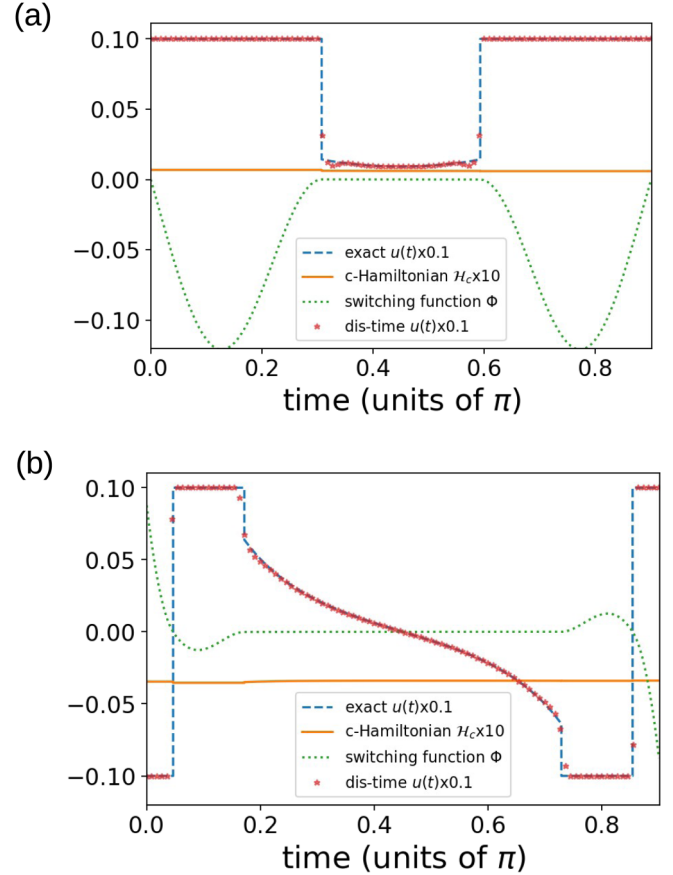

FIG. 1. The optimal controls (dashed curves) for (a) the state-retention and (b) state-preparation problems. A bang control corresponds to nonzero Φ (dotted curves), whereas a singular control corresponds to the vanishing Φ. The exact optimal controls (dashed curves) are obtained using the formalism developed in Ref. [40]. The c-Hamiltonian (solid curves) is a constant over the entire evolution time t_f. The dotted curves are the numerical solutions obtained using the gradient-based method with the switching function computed by solving the Lindbladian equation; good agreement is seen.

explicit constructions of the density matrix and its costates. Using the optimal control for the state-retention problem [given in Fig. 1(a)], we compute ρ [Eq. (16)], λ [Eq. (18)], and thus Φ [Eq. (9)] and $\mathcal{H}_c$ [Eq. (10) and (13)]. The results are shown in Fig. 2 and agree well with the exact results (i.e., the results from the deterministic Lindbladian formalism). Note that in Fig. 2(c), Φ and $\mathcal{H}_c$ display larger errors around the switching times; we have tested that this discrepancy becomes weaker upon increasing the time points (not shown). To test the second procedure, Fig. 3 compares the switching functions computed using Eq. (22) with the exact ones. In these simulations, the nonoptimal control $u(t) = -1 + 2\Theta(t - t_f/2)$ is used. Good agreement is seen for both state-retention and state-preparation problems, numerically confirming Eq. (22).

C. Optimal control

With the switching functions tested, Eq. (22) is now applied to determine the optimal control for both state-retention and state-preparation problems. Due to the noisy nature of
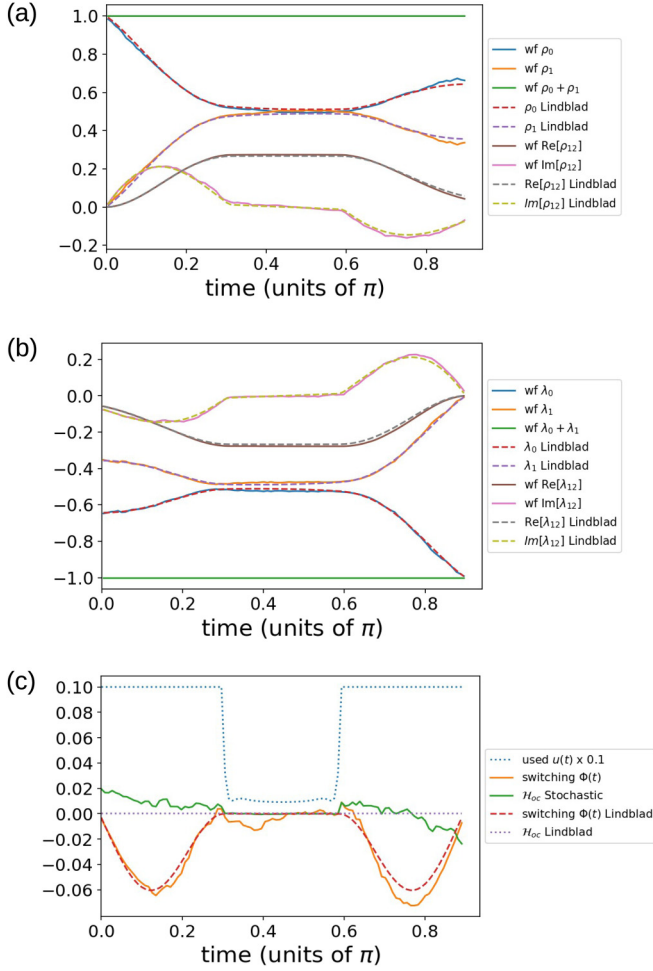
FIG. 2. Comparison between the deterministic Lindbladian (dashed curves) and the stochastic Schrödinger (solid curves) simulations for (a) the density matrix ρ and (b) the costate density matrix λ. The control is chosen to be the optimal control for the state-retention problem [dotted curve in (c)]. The stochastic results use 100 time points and average over 500 realizations. (c) Combination of ρ and λ to evaluate the switching function and c-Hamiltonian.

stochastic simulations, filtering the functions at some point helps. After some numerical experiments, we adopt two filtering protocols: the $(k + 1)$th iteration is updated via

$$\tilde{u}^{(k+1)}(t) \leftarrow u^{(k)}(t) - \eta \, \tilde{\Phi}^{(k)}(t), \tag{26a}$$

$$u^{(k+1)}(t) \leftarrow P_\varepsilon[\tilde{u}^{(k+1)}(t)]. \tag{26b}$$

We first elaborate Eq. (26a). After $\Phi^{(k)}(t)$ is computed from Eq. (22), it is denoised by a total-variation (TV) norm [68]:

$$\tilde{\Phi}^{(k)}(t) = \underset{y(t)}{\mathrm{argmin}} \sum_{t_i} \left[\frac{1}{2} \{y(t_i) - \Phi^{(k)}(t_i)\}^2 \right.$$

$$\left. + w_{TV} \|y(t_{i+1}) - y(t_i)\| \right\}. \tag{27}$$

$w_{TV} = 0.01$ is adopted, and the proximal gradient descent is used to solve Eq. (27). We decide to regularize $\Phi(t)$ instead of
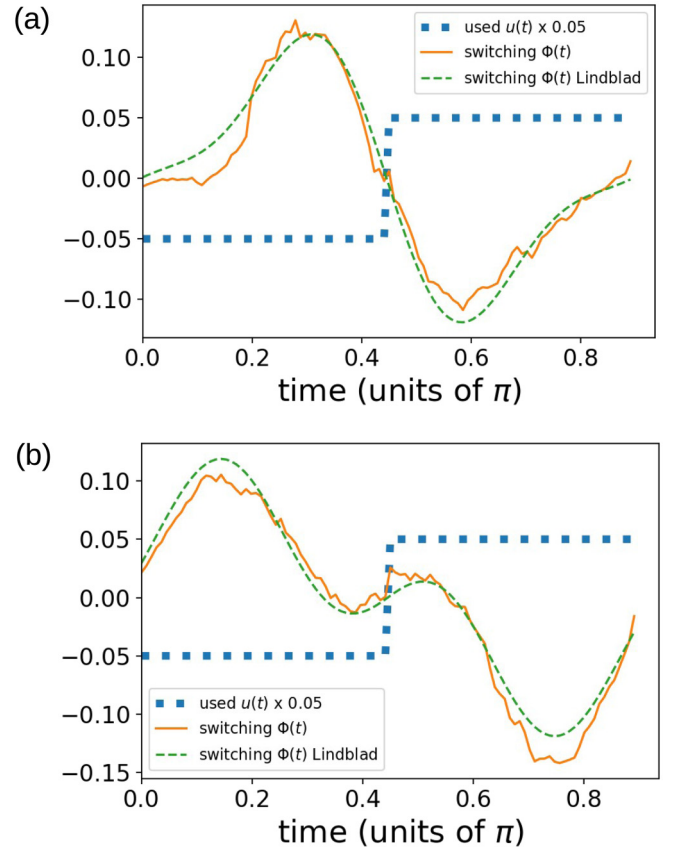

FIG. 3. The switching function computed using the Lindbladian formalism [Eq. (9), dashed curves] and using the stochastic procedure described by Eq. (22) (solid curves, averaging over 500 simulations). Blue dotted curves specify $u(t)$. The initial and target states are (a) the state-retention problem [Eq. (24)] and (b) the state-preparation problem [Eq. (25)].

$u(t)$ because the TV norm tends to reduce the magnitude of the discontinuity (jump): there will be a discontinuity in $u(t)$ once $\Phi(t)$ changes sign (the bang-bang protocol), whereas $\Phi(t)$ is generally continuous. In Eq. (26b), the projection P_ε is defined as

$$P_\varepsilon[u(t)] \equiv \begin{cases} 1 & \text{if } u(t) > 1 - \varepsilon, \\ -1 & \text{if } u(t) < -(1 - \varepsilon). \end{cases} \tag{28}$$

$\epsilon = 0.1$ is used. This is designed to promote the bang control around $\Phi(t) = 0$. We choose $\varepsilon = 0$ in early iterations to avoid biases when $u(t)$ is still far from the optimal solution. To summarize, three optimization hyperparameters are chosen to be $(\eta, w_{TV}, \varepsilon) = (0.5, 0.01, 0.1)$.

Figures 4(a) and 4(c) show the optimal control obtained using Eq. (22) for both the state-retention and state-preparation problems. They generally agree with the exact solutions. Compared to the solutions without filtering ($w_{TV} = \varepsilon = 0$), the filtering procedure generally results in controls that are smoother over the singular regime [when $\Phi(t) = 0$] and sharper near the transition regimes [when $\Phi(t)$ changes sign or changes between zero and nonzero]. Overall, the controls with the filtering procedure are closer to the exact solutions. Figures 4(b) and 4(d) give the negative of terminal cost
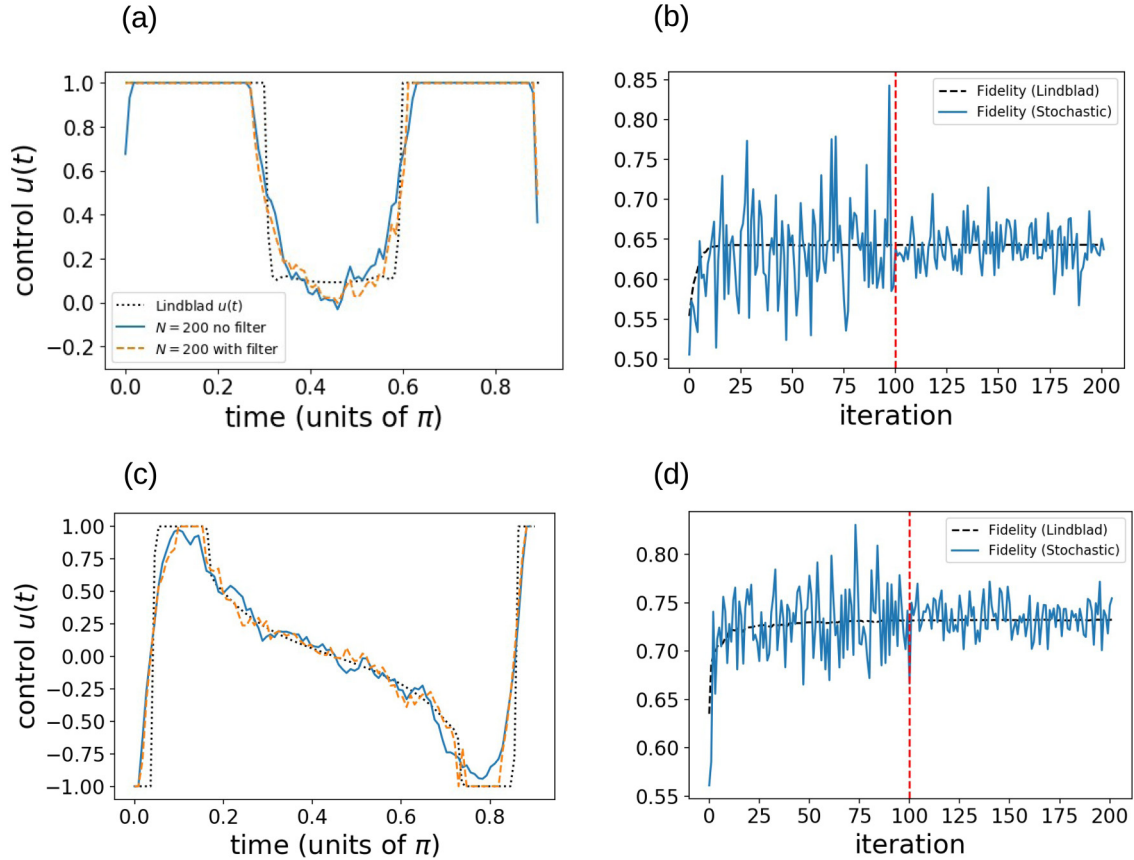
FIG. 4. Results of (a) and (b) state-retention and (c) and (d) state-preparation problems. (a) and (c) Compared to the optimal controls without filtering (solid curves), the optimal controls with the filtering procedure [Eq. (26), dashed curves] are closer to those obtained from the Lindbladian formalism (dotted curves). (b) and (d) The fidelities computed from the deterministic Lindbladian [Eq. (9), dashed curves] and the stochastic Schrödinger [Eq. (20), solid curves] formalisms. The values agree well. In the stochastic simulations, the first 100 iterations average 50 realizations, whereas the last 100 average 200 (separated by the red vertical line). The expected fluctuation reduction due to the larger sampling size is clearly seen.

function (fidelity) as a function of iterations. The fidelities computed from the deterministic Lindbladian [Eq. (9), dashed curves] and the stochastic Schrödinger [Eq. (20), solid curves] formalisms are numerically consistent. For the stochastic simulation, the first 100 iterations average $N = 50$ realizations, whereas the last 100 iterations average $N = 200$. The expected reduction of the fluctuation due to the larger sampling size is also clearly seen.

V. CONCLUSION

A quantum task was mapped to an optimal-control problem once a proper terminal cost function was defined. In terms of optimal control, an optimal solution extremizes the cost function for a given evolution time, and practically, the most crucial step to determine the optimal control is the evaluation of the gradient of the terminal cost function. Using PMP, the gradient was efficiently obtained by calculating the switching function that requires solving the original dynamical problem and an auxiliary problem composed of costate variables. In this work, we formulated PMP in terms of density matrices

which are essential for open quantum systems and developed a stochastic procedure to compute the switching function for systems obeying Lindbladian dynamics. In particular, we determined the rules to consistently update the wave function and its costate in the stochastic Schrödinger formalism so that the switching function can be evaluated without explicitly constructing density matrices. We apply the proposed procedure to determine the optimal control for a dissipative qubit system, and the results are consistent with those obtained directly from the deterministic Lindbladian equation. The proposed formalism saves time and memory for simulating large systems and can be straightforwardly generalized to describe non-Markovian dynamics.

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