Efficient Optimal Control of Open Quantum Systems

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Abstract

The optimal control problem for open quantum systems can be formulated as a time-dependent Lindbladian that is parameterized by a number of time-dependent control variables. Given an observable and an initial state, the goal is to tune the control variables so that the expected value of some observable with respect to the final state is maximized. In this paper, we present algorithms for solving this optimal control problem efficiently, i.e., having a poly-logarithmic dependency on the system dimension, which is exponentially faster than best-known classical algorithms. Our algorithms are hybrid, consisting of both quantum and classical components. The quantum procedure simulates time-dependent Lindblad evolution that drives the initial state to the final state, and it also provides access to the gradients of the objective function via quantum gradient estimation. The classical procedure uses the gradient information to update the control variables.

At the technical level, we provide the first (to the best of our knowledge) simulation algorithm for time-dependent Lindbladians with an ℓ_1-norm dependence. As an alternative, we also present a simulation algorithm in the interaction picture to improve the algorithm for the cases where the time-independent component of a Lindbladian dominates the time-dependent part. On the classical side, we heavily adapt the state-of-the-art classical optimization analysis to interface with the quantum part of our algorithms. Both the quantum simulation techniques and the classical optimization analyses might be of independent interest.

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1 Introduction

The ability to control the dynamics of a quantum system to maximize its property has been a persistent pursuit in quantum physics and chemistry [18]. This endeavor has recently gained momentum, spurred by the growing interest in designing quantum information processing devices. One remarkable obstacle in controlling a quantum system's behavior stems from the reality that quantum systems typically evolve in the presence environmental noise. Consequently, the control strategy must take into account system/bath interactions. In the Markovian regime, this problem can be formulated as an optimal control problem based on the Lindblad master equation [38, 24] acting on n qubits,

$$\frac{d}{dt}\rho = \mathcal{L}(t)(\rho) := -i\left[H_0 + \sum_{\beta=1}^{n_c} u_\beta(t)\mu_\beta, \rho\right] + \sum_{j=1}^{m}\left(L_j\rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\}\right), \tag{1}$$

in conjunction with a control functions $u_\beta(t)$ that enters the system Hamiltonian through the operator μ_β, and we have n_c control functions. Here ρ is a density operator on n qubits, and the second term in Eq. (1) is a result of system/bath interactions with L_j's being the jump operators. The quantum optimal control (QOC) is then formulated as an optimization problem following [2]:

$$\max_{\boldsymbol{u}} f[\boldsymbol{u}(t)], \quad f[\boldsymbol{u}(t)] \coloneqq \mathrm{tr}\big(\mathcal{O}\rho(T)\big) - \alpha\sum_{\beta=1}^{n_c}\int_0^T |u_\beta(t)|^2 \mathrm{d}t. \tag{2}$$

The Hermitian operator $\mathcal{O}$ represents the property to be maximized. The term $\boldsymbol{u}(t)$ embodies all the control variables $\{u_\beta\}$ and the last term in the objective function $f[\boldsymbol{u}(t)]$ is regarded as a regularization. It is worthwhile to point out that there are other choices of the objective function [8] in the formulation of the QOC problem. For example, one can guide the Lindblad dynamics (1) toward a target state $\bar{\rho}(T)$. In this case, one can minimize the difference between $\bar{\rho}(T)$ and $\rho(T)$,

$$\min_{\boldsymbol{u}} f[\boldsymbol{u}(t)], \quad f[\boldsymbol{u}] := \|\rho(T) - \bar{\rho}(T)\|^2 + \alpha\sum_{\beta}\int_0^T |u_\beta(t)|^2 \mathrm{d}t. \tag{3}$$

Implicit in both optimization problems Eqs. (2) and (3) is that $\rho(T)$ has to be obtained from the Lindblad equation (1). Thus the main computational challenge comes from the repeated computation of the solution of the Lindblad equation. In this paper, we mainly focus on the optimal control problem with the objective function Eq. (2).

To be able to clearly illustrate the computational complexity, we assume that the Hamiltonian $H(t)$ and the jump operators $L_j(t)$'s are sparse. Moreover, the sparsity structure for each operator does not change over time (i.e., the positions of nonzero entries do not change with time). For a sparse matrix A, we assume we have access to a procedure $\mathcal{P}_A$ that can apply the following oracles:

$$\mathcal{O}_{A,\mathrm{loc}}|i,j\rangle = |i,\nu_A(i,j)\rangle, \quad \text{and} \tag{4}$$

$$\mathcal{O}_{A,\mathrm{val}}|t,i,j,z\rangle = |t,i,j,z\oplus A_{i,j}(t)\rangle, \tag{5}$$

where $\nu_A(i,j)$ is the index of the j's nonzero entry of column i in A. Particularly for the optimal control problem, we assume we have access to $\mathcal{P}_{H_0}$, $\mathcal{P}_{\mu_\beta}$, and $\mathcal{P}_{L_j}$ for all $j \in [m]$, as well as $\mathcal{P}_{\mathcal{O}}$ for the observable $\mathcal{O}$.

Main contributions

We will present a hybrid quantum/classical algorithm for the QOC problem (1) and (2). The overall algorithm consists of the following elements:

1. A Lindblad simulation algorithm [14, 15, 36] that prepares $\rho(T)$ in a purification form. The complexity of our algorithm exhibits a linear scaling with respect to T with a scaling factor proportional to the L_1 norm of the Lindbladians instead of the $L_{\max}$ norm. The dependence of the complexity on the precision ϵ is only poly-logarithmic. Alternatively, we can also simulate time-dependent Lindbladian using interaction picture [41]. This algorithm applies to important models in experimental physics. For instance, in an ion trap system, it is common to have a time-independent Hamiltonian with norm much larger than the rest of the Lindbladian terms, and thus our algorithm can make the simulation more efficient.
2. The construction of a quantum phase oracle of the gradient of the function f. This is achieved by incorporating the quantum gradient computation algorithms in [21]. This phase oracle will then be interfaced with a classical optimization algorithm.
3. Having approximates of gradients $\nabla f(\boldsymbol{u}(t))$, we use an accelerated gradient descent (AGD) method [27] to solve the optimization problem. In particular, we analyze the influence of the statistical error from the gradient estimation and provide a precise complexity analysis for solving the optimization problem, which essentially characterizes the robustness of AGD for reaching second-order stationary points and may be of independent interest.

In addition to the proposed algorithms, we provide rigorous analysis of the numerical error and precise overall complexity estimates for the hybrid algorithm. Formally, we establish the following result for optimal control of open quantum systems:

▶ **Theorem 1** (main theorem). *Assume there are n_c control functions $u_\beta(t) \in \mathrm{C}^2([0,T])$. Further assume*[1] *that $\|H_0\|, \|\mathcal{O}\|, \|\mu_\beta\|, \|L_j\| \le 1$, and $\alpha \ge 2/T$. There exists a quantum algorithm that, with probability at least $2/3$*[2]*, solves problem (2) by:*

- *reaching a first-order stationary point $\|\nabla f\| < \epsilon$ with (1) using $\widetilde{O}\left(\frac{n_c\|\mathcal{L}\|_{be,1}T}{\epsilon^{23/8}}\Delta_f\right)$ queries to $\mathcal{P}_{H_0}$ and $\mathcal{P}_{\mu_\beta}$, $\beta = 1,2,\ldots,n_c$, and $\widetilde{O}\left(mn\frac{n_c\|\mathcal{L}\|_{be,1}T}{\epsilon^{23/8}}\Delta_f + n\frac{T^{3/2}}{\epsilon^{9/4}}\Delta_f\right)$ additional 1- and 2-qubit gates; or*
- *reaching a second-order stationary point using $\widetilde{O}\left(\frac{n_c\|\mathcal{L}\|_{be,1}T^{7/4}}{\epsilon^{5}}\Delta_f\right)$ queries to $\mathcal{P}_{H_0}$ and $\mathcal{P}_{\mu_\beta}$, $\beta = 1,2,\ldots,n_c$ and $\widetilde{O}\left(mn\frac{n_c\|\mathcal{L}\|_{be,1}T^{7/4}}{\epsilon^{5}}\Delta_f + n\frac{T^{3/2}}{\epsilon^{9/4}}\Delta_f\right)$ additional 1- and 2-qubit gates.*

Here n_c and m are respectively the number of control variables and jump operators.

Techniques

Our technical contributions are outlined as follows.

[1] More generally, if $\|H_0\|, \|\mu\| = \Theta(\Lambda)$, it is equivalent to enlarge the time duration T by a factor $O(\Lambda)$.
[2] Using standard techniques, the success probability can be boosted to a constant arbitrarily close to 1 while only introducing a logarithmic factor in the complexity.

- In Section 3, we give efficient quantum algorithms for simulating time-dependent Lindbladians with a scaling factor in time proportional to the L_1-norm of the Lindbladians instead of the $L_{\max}$-norm, as well as poly-logarithmic ϵ dependence. Our simulation algorithm is based on the higher-order series expansion from Duhamel's principle as sketched in [36]. A notable difference from [36] is that in their paper, Gaussian quadratures are used to approximate integrals; however, in our time-dependent case, Gaussian quadratures can no longer be used as, unless upper bounds on the higher-order derivatives of the operators are given in advance. The techniques for obtaining the L_1-norm dependence follow from the rescaling trick in [5], while generalized to Lindbladians. Our time-dependent Lindbladian simulation techniques might be of independent interest.
- In Section 4, we show how to simulate time-dependent Lindbladian using interaction picture [41]. This technique is suited for simulating a Lindbladian $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ where $\mathcal{L}_1(\cdot) = -i\,[H_1, \cdot]$ is a Hamiltonian with complexity linear in norm of $\mathcal{L}_2$ (up to poly-logarithmic factors) and similar number of simulations of the Hamiltonian H_1 . The simulation scheme is based on a mathematical treatment of the Lindblad equation as a differential equation, and the construction leverages the simulation algorithms shown in Section 3 without rescaling the evolution time. It turns out that using our simulation algorithm in the interaction picture, we obtain better gate complexity compared with directly using the simulation in Section 3 even with the ℓ_1-norm dependence. To the best of our knowledge, this is the first Lindblad simulation algorithm in the interaction picture, which can also be of independent interest.
- In Section 5, we adapt a nonconvex optimization algorithm that can reach first-order stationary points with $\tilde{O}(1/\epsilon^{7/4})$ *noisy* gradient queries with ℓ_2-norm error at most $O(\epsilon^{9/8})$, and reach second-order stationary points with $\tilde{O}(1/\epsilon^{7/4})$ *noisy* gradient queries with ℓ_2-norm error at most $\tilde{O}(\epsilon^3)$. Our setting is different from either gradient descent (GD) or stochastic gradient descent (SGD): Compared to GD we only have access to noisy gradients, while in standard SGD the noise can be adjusted and there is no Lipschitz condition for the noisy gradient. With this novel setting, we successfully design an optimization algorithm based on perturbed accelerated gradient descent (PAGD) [27]. We carefully analyze the error bound in different cases and it turns out that our algorithm reaches an optimal error scaling for PAGD (up to poly-logarithmic factors) in finding a first-order stationary point.

Related work

In addition to the large variety of conventional applications [20], quantum optimal control problems are crucial in near-term quantum computing, because in the architecture of quantum computers, the underlying physical operations such as microwave control pulses and the modulated laser beam can be abstracted as control pulse sequences (see the survey [47] for more detailed discussions), and hence the are inherently quantum control problems. Quantum optimal control also plays a vital role in quantum computing algorithms. For instance, Magann et al. [42] studied the relationship between variational quantum algorithms (VQAs) and quantum optimal control, and showed that the performance of VQAs can be informed by quantum optimal control theory. Banchi and Crooks [4] demonstrated how gradients can be estimated in a hybrid quantum-classical optimization algorithm, and quantum control is used as one important application. In Ref. [40] the authors showed that for a quantum many-body system, if it exists an efficient classical representation, then the optimal control problems on this quantum dynamics can be solved efficiently with finite precision.

There exist heuristic classical methods for solving the quantum optimal control problem, including the monotonically convergence algorithms [48], the Krotov method [45], the GRadient Ascent Pulse Engineering (GRAPE) algorithm [29, 17], the Chopped RAndom-Basis (CRAB) algorithm [9], etc. Furthermore, such heuristics can be extended to quantum optimal control of open quantum systems [31, 32, 46, 23], including [1, 33, 6]. However, these algorithms do not establish provable guarantees for the efficiency of solving the quantum optimal control problem. Meanwhile, the landscape of the quantum control problem has been analyzed in [13, 16, 19], which suggests that for closed quantum systems, the landscape may not involve suboptimal optimizers. However, the implication to the computational complexity still remains open.

Quantum algorithms, due to their natural ability to simulate quantum dynamics, have been developed for quantum control problems [43, 34, 12, 35]. Liu and Lin [39] developed an efficient algorithm to output the integral of the observable in Eq. (2), which can potentially solve a more generalized optimal control problem. These approaches employ hybrid quantum-classical algorithms that combine a quantum algorithm for the time-dependent Schrödinger equation with a classical optimization method. However, these efforts have been focused on closed quantum systems, and quantum control algorithms for open quantum systems require separate techniques.

Open questions

Our paper leaves several open questions for future investigations:

- Are there efficient quantum algorithms for the optimal control of other master equations beyond the Lindbladian equation?
- How to extend the current framework to the control problems with a target density operator $\bar{\rho}(T)$? The challenge in such a control problem (3) is the estimation of the Frobenius norm from the quantum circuit.
- Gaussian quadrature was used in the Lindblad simulation method [36], which significantly suppressed the number of terms in a Dyson-series type of approach, and implies the implementation. The extension of Gaussian quadrature to the current framework with time-dependent Lindbladians would require derivative bounds for the evolution operator from both the drift and jump terms, which is not trivial.

2 Preliminaries

2.1 Notations

For a positive integer m, we use $[m]$ to denote the set $\{1, \ldots, m\}$. In this paper, we use two types of notations to denote vectors. For a quantum state, we use the Dirac notation $|\cdot\rangle$ to denote the corresponding state vector. For vectors involved in classical information, e.g., the gradient vector, we use bold font, such as $\boldsymbol{u}$, to denote them. For such a vector $\boldsymbol{u} \in \mathbb{C}^d$, we use subscripts with a norm font to indicate its entries, i.e., $u_1, \ldots, u_d$ are the entries of $\boldsymbol{u}$. When we use subscripts with a bold font, such as, $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k$, they are a list of vectors. For a vector $\boldsymbol{v} \in \mathbb{C}^d$, we use $\|\boldsymbol{v}\|$ to denote its *Euclidean norm*. For a matrix $M \in \mathbb{C}^{d\times d}$, we use $\|M\|$ to denote its *spectral norm*, and use $\|M\|_1$ to denote its *trace norm*, i.e., $\|A\|_1 = \mathrm{Tr}(\sqrt{M^\dagger M})$. We also use $[\cdot,\cdot]$ to denote the operator *commutator*, i.e., $[A, B] \coloneqq AB - BA$, and use $\{\cdot,\cdot\}$ to denote the *anticommutator*, i.e., $\{A, B\} \coloneqq AB + BA$.

In addition, we use calligraphic fonts, such as $\mathcal{L}$, to denote *superoperators*, which is also referred to as *quantum maps*. Superoperators are linear maps that take matrices to matrices. The *induced trace norm* of a superoperator $\mathcal{M}$, denoted by $\|\mathcal{M}\|_1$, is defined as

$$\|\mathcal{M}\|_1 \coloneqq \max\{\|\mathcal{M}(A)\|_1 : \|A\|_1 \leq 1\}. \tag{6}$$

The *diamond norm* of a superoperator $\mathcal{M}$, denoted by $\|\mathcal{M}\|_\diamond$, is defined as

$$\|\mathcal{M}\|_\diamond \coloneqq \|\mathcal{M} \otimes \mathcal{I}\|_1, \tag{7}$$

where $\mathcal{I}$ acts on the space with the same size as the space $\mathcal{M}$ acts on.

We denote by $\mathrm{C}^2[0,T]$ the class of twice continuously differential functions in $[0,T]$.

2.2 Algorithmic tools

2.2.1 Block-encoding and implementing completely-positive maps

Although we assume that the input of the operators of the Lindbladian are given by sparse-access oracles, it is convenient to use a more general input model when presenting the simulation algorithm. For a matrix $A \in \mathbb{C}^{2^n \times 2^n}$, we say that a unitary, denoted by U_A, is an (α, b, ϵ)-block-encoding of A if $\|A - \alpha(\langle 0|^{\otimes b} \otimes I) U_A (|0\rangle^{\otimes b} \otimes I)\| \leq \epsilon$, where the identity operator I is acting on n qubits. Intuitively, this unitary U_A is acting on $(n+b)$ qubits and A appears in the upper-left block of it, i.e., $U_A = \begin{pmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{pmatrix}$. Here, we refer to α as the *normalizing factor*.

Our simulation algorithm relies on the following technical tool from [37] for implementing completely positive maps given the block-encodings of its Kraus operators, which generalizes a similar tool in [15] where the Kraus operators are given as linear combinations of unitaries.

▶ **Lemma 2** (Implementing completely positive maps via block-encodings of Kraus operators [37]). *Let $A_1, \ldots, A_m \in \mathbb{C}^{2^n}$ be the Kraus operators of a completely positive map. Let $U_1, \ldots, U_m \in \mathbb{C}^{2^{n+n'}}$ be their corresponding (s_j, n', ϵ)-block-encodings, i.e.,*

$$\|A_j - s_j(\langle 0| \otimes I) U_j (|0\rangle \otimes I)\| \leq \epsilon, \quad \text{for all } 1 \leq j \leq m. \tag{8}$$

Let $|\mu\rangle \coloneqq \frac{1}{\sqrt{\sum_{j=1}^m s_j^2}} \sum_{j=1}^m s_j |j\rangle$. Then $(\sum_{j=1}^m |j\rangle\langle j| \otimes U_j) |\mu\rangle |0\rangle \otimes I$ implements this completely positive map in the sense that

$$\left\| I \otimes \langle 0| \otimes I \left(\sum_{j=1}^m |j\rangle\langle j| \otimes U_j \right) |\mu\rangle |0\rangle |\psi\rangle - \frac{1}{\sqrt{\sum_{j=1}^m s_j^2}} \sum_{j=1}^m |j\rangle A_j |\psi\rangle \right\| \leq \frac{m\epsilon}{\sqrt{\sum_{j=1}^m s_j^2}} \tag{9}$$

for all $|\psi\rangle$.

We also need the following lemma from [37] for obtaining a block-encoding of a linear combination of block-encodings.

▶ **Lemma 3** (Block-encoding of a sum of block-encodings [37]). *Suppose $A \coloneqq \sum_{j=1}^m y_j A_j \in \mathbb{C}^{2^n \times 2^n}$, where $A_j \in \mathbb{C}^{2^n \times 2^n}$ and $y_j > 0$ for all $j \in \{1, \ldots m\}$. Let U_j be an (α_j, a, ϵ)-block-encoding of A_j, and B be a unitary acting on b qubits (with $m \leq 2^b - 1$) such that $B|0\rangle = \sum_{j=0}^{2^b-1} \sqrt{\alpha_j y_j / s} |j\rangle$, where $s = \sum_{j=1}^m y_j \alpha_j$. Then a $(\sum_j y_j \alpha_j, a+b, \sum_j y_j \alpha_j \epsilon)$-block-encoding of $\sum_{j=1}^m y_j A_j$ can be implemented with a single use of $\sum_{j=0}^{m-1} |j\rangle\langle j| \otimes U_j + ((I - \sum_{j=0}^{m-1} |j\rangle\langle j|) \otimes I_{\mathbb{C}^{2^a}} \otimes I_{\mathbb{C}^{2^n}})$ plus twice the cost for implementing B.*

2.2.2 Optimization

For the current quantum-classical hybrid algorithm, we will couple a Lindblad simulation with a classical optimization algorithm. For this purpose, we work with the PAGD algorithm [27], which is based on Nesterov's accelerated gradient descent idea [44],

$$\boldsymbol{u}_{k+1} = \boldsymbol{u}_k - \eta \nabla f(\boldsymbol{u}_k) + (1-\theta)\boldsymbol{v}_k, \quad \boldsymbol{v}_{k+1} \quad = \boldsymbol{u}_{k+1} - \boldsymbol{u}_k. \tag{10}$$

Here $\boldsymbol{u}_k$ is the kth iterate of the control variable. The idea in PAGD is to introduce a perturbation to the iterate when $\|\nabla f\| > \epsilon$ for some iterations, along with a negative curvature exploitation step.

There are two common goals for solving (nonconvex) optimization problems:

- $\boldsymbol{x}$ is called an ϵ-approximate first-order stationary point if $\|\nabla f(\boldsymbol{x})\| \leq \epsilon$.
- $\boldsymbol{x}$ is called an ϵ-approximate second-order stationary point if $\|\nabla f(\boldsymbol{x})\| \leq \epsilon$, $\lambda_{\min}(\nabla^2 f(\boldsymbol{x})) \geq -\sqrt{\varrho\epsilon}$. Here f is a ϱ-Hessian-Lipschitz function, i.e., $\|\nabla^2 f(\boldsymbol{x}) - \nabla^2 f(\boldsymbol{y})\| \leq \varrho\|\boldsymbol{x} - \boldsymbol{y}\|$ for any $\boldsymbol{x}$ and $\boldsymbol{y}$.

2.2.3 Quantum gradient estimation

With copies of $\rho(T)$, which will be obtained from Lindblad simulation algorithms, and sparse access to $\mathcal{O}$, we can obtain an estimated gradient value of $\widetilde{J}_1(\boldsymbol{u})$. The high-level strategy is to construct a probability oracle first, then construct a phase oracle with the probability oracle, and finally obtain the gradient by the phase oracle. The probability oracle and the phase oracle are defined as follows.

The Lindblad simulation algorithm leads to a purification of $\rho(T)$, i.e., $\rho(T) = \mathrm{tr}(|\rho_T\rangle\langle\rho_T|)$. It is clear that the regularization term in (2) is easy to compute. With the purification, we can express the first term as,

$$\widetilde{J}_1(\boldsymbol{u}) := \langle\rho_T|\, \mathcal{O} \otimes I\, |\rho_T\rangle\,. \tag{11}$$

Suppose $U_{\mathcal{O}}$ denotes the block encoding of $\mathcal{O}$, i.e. $\langle 0\,|\langle\psi_N\,|U_{\mathcal{O}}|\,0\rangle|\,\psi_N\rangle = \langle\psi_N|\mathcal{O}|\psi_N\rangle$. Let c-$U_{\mathcal{O}}$ be the controlled $U_{\mathcal{O}}$. Applying Hadamard test circuit $(H \otimes I)\,(\mathrm{c}{-}U_{\mathcal{O}})\,(H \otimes I)$ acting on $|\rho_T\rangle$ produces

$$\sqrt{f(\boldsymbol{u})}\,|1\rangle\,|\phi_1(u)\rangle + \sqrt{1 - f(\boldsymbol{u})}\,|0\rangle\,|\phi_0(\boldsymbol{u})\rangle \tag{12}$$

where $f(\boldsymbol{u}) := -\frac{1}{2}\langle\rho_T|\mathcal{O}|\rho_T\rangle + \frac{1}{2} = -\frac{1}{2}\widetilde{J}_1(\boldsymbol{u}) + \frac{1}{2}$. By Lemma 48 of [22], we can efficiently construct a block encoding of $\mathcal{O}$ with sparse access to $\mathcal{O}$. The $1/2$ factor does not matter because the gradient will only be multiplied by a constant factor.

▶ **Definition 4** (Probability oracle). *Consider a function $f : \mathbb{R}^d \to [0,1]$. The probability oracle for f, denoted by U_f, is a unitary defined as*

$$U_f|\boldsymbol{x}\rangle|\boldsymbol{0}\rangle = |\boldsymbol{x}\rangle\left(\sqrt{f(\boldsymbol{x})}|1\rangle\,|\phi_1(\boldsymbol{x})\rangle + \sqrt{1 - f(\boldsymbol{x})}|0\rangle\,|\phi_0(\boldsymbol{x})\rangle\right),$$

where $|\phi_1(\boldsymbol{x})\rangle$ and $|\phi_0(\boldsymbol{x})\rangle$ are arbitrary states.

▶ **Definition 5** (Phase oracle). *Consider a function $f\colon \mathbb{R}^d \to \mathbb{R}$. The phase oracle for f, denoted by $\mathcal{O}_f$, is a unitary defined as*

$$\mathcal{O}_f|\boldsymbol{x}\rangle|\boldsymbol{0}\rangle = e^{if(\boldsymbol{x})}|\boldsymbol{x}\rangle|\boldsymbol{0}\rangle$$

▶ **Theorem 6** (Constructing phase oracle with probability oracle, Theorem 14 of [21]). *Consider a function $f : \mathbb{R}^d \to [0,1]$. Let U_f be the probability oracle for f. Then, for any $\epsilon \in (0, 1/3)$, we can implement an ϵ-approximate of the phase oracle $\mathcal{O}_f$ for f, denoted by $\widetilde{\mathcal{O}}_f$, such that $\|\widetilde{\mathcal{O}}_f|\psi\rangle|\boldsymbol{x}\rangle - \mathcal{O}_f|\psi\rangle|\boldsymbol{x}\rangle\| \leq \epsilon$, for all state $|\psi\rangle$. This implementation uses $O(\log(1/\epsilon))$ invocations to U_f and $U_f^\dagger$, and $O(\log\log(1/\epsilon))$ additional qubits.*

In order to interface the Lindblad simulation algorithm with a classical optimization method, one needs to estimate the gradient of the objective function. Similar to the approach in [35], we first represent the control variable as a piecewise linear function in time

$u_\beta(t) \approx \sum_{j=1}^{N} u_j B_j(t)$ with $B_j(t)$ being the standard shape function and u_j being a nodal function. The total number of steps N is proportional to the time duration T. We will use the improved Jordan's algorithm [28] using high order finite difference formulas [21]. Basically, the gradient estimation in [21] produces an estimate $\boldsymbol{g}(\boldsymbol{u})$, such that, $\|\nabla J_1(\boldsymbol{u}) - \boldsymbol{g}(\boldsymbol{u})\| < \epsilon$ with complexity $O(d/\epsilon)$, which is clearly better than a direct sampling approach. However, to achieve this complexity, the objective function needs to satisfy a derivative bound. Toward this end, we first establish an a priori bound for the derivative.

▶ **Lemma 7.** *Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_k) \in [N+1]^k$ be an index sequence[3]. The derivatives of the control function $\widetilde{J}_1$ with respect to the control variables satisfy:*

$$\left\| \frac{\partial^{\boldsymbol{\alpha}} \widetilde{J}_1}{\partial u_{\alpha_1} u_{\alpha_2} \cdots u_{\alpha_k}} \right\| \leq (k+1)! \left(\delta t \|\mu\|\right)^k . \tag{13}$$

This smoothness provides a basis for estimating the complexity of Jordan's algorithm [21],

▶ **Lemma 8** (Rephrased from Theorem 23 of [21])**.** *Suppose the access to $f\colon [-1,1]^N \to \mathbb{R}$ is given via a phase oracle O_f. If f is $(2m+1)$-times differentiable and for all $\boldsymbol{x} \in [-1,1]^N$, and $|\partial_{\boldsymbol{r}}^{2m+1} f(\boldsymbol{x})| \leq B$ for $\boldsymbol{r} = \boldsymbol{x}/\|\boldsymbol{x}\|$, then there exists a quantum algorithm that outputs an approximate gradient $\boldsymbol{g}$ such that $\|\boldsymbol{g} - \nabla f(\boldsymbol{0})\|_\infty \leq \epsilon$ with probability at least $1-\rho$ using*

$$\widetilde{O}\left(\max\left\{\frac{N^{1/2} B^{1/(2m)} N^{1/(4m)} \log(N/\rho)}{\epsilon^{1+1/(2m)}}, \frac{m}{\epsilon}\right\}\right) \tag{14}$$

queries to O_f, and $\widetilde{O}(N)$ additional 1- and 2-qubit gates.

In particular, when $f(\boldsymbol{x})$ is a polynomial of degree no greater than $2m$, the query complexity to O_f becomes, $\widetilde{O}\left(\frac{m}{\epsilon}\right)$.

After adapting this algorithm to the objective function in Eq. (11), we find that,

▶ **Lemma 9.** *Let $\widetilde{J}_1$ be defined as in Eq. (11). Suppose we are given access to the phase oracle $\mathcal{O}_{\widetilde{J}_1}$ for $\widetilde{J}_1$. Then, there exists a quantum algorithm that outputs an approximate gradient $\boldsymbol{g}$ such that $\|\boldsymbol{g} - \nabla \widetilde{J}_1\| \leq \epsilon_g$ with probability at least $1-\gamma$ using $\widetilde{\mathcal{O}}\left(n_c T \log(N/\gamma)/\epsilon_g\right)$ queries to $\mathcal{O}_{\widetilde{J}_1}$, and $\widetilde{O}(N)$ additional 1- and 2-qubit gates.*

Proof. Although the derivative bound in Lemma 7 does not fulfill the condition in [21], we can apply Theorem 23 in [21]. By choosing the optimal value m, we arrive at the complexity bound. ◀

With the gradient estimated, we can now move to the optimization algorithm. The PAGD algorithm in [27] assumes the gradient- and Hessian-Lipschitz condition, which we will prove here for the control problem. In particular, the smoothness constant ℓ and the Hessian-Lipschitz constant ϱ can be approximated by the same technique as Lemma 7.

▶ **Lemma 10.** *Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_k) \in [N+1]^k$ be an index sequence, then $\tilde{J}_1$ is l-smooth and ρ-Hessian Lipschitz continuous, i.e.*

$$\|\boldsymbol{\nabla} \tilde{J}_1(\boldsymbol{u}) - \boldsymbol{\nabla} \tilde{J}_1(\boldsymbol{v})\| \leq l\|\boldsymbol{u} - \boldsymbol{v}\|, \text{and} \quad \|\boldsymbol{\nabla}^2 \tilde{J}_1(\boldsymbol{u}) - \boldsymbol{\nabla}^2 \tilde{J}_1(\boldsymbol{v})\| \leq \varrho\|\boldsymbol{u} - \boldsymbol{v}\|. \tag{15}$$

The smoothness parameters are given by, $l = 3!(N+1)\delta t^2 \|\mu\|^2 \|\mathcal{O}\|$, $\quad \varrho = 4!(N+1)\delta t^3 \|\mu\|^3 \|\mathcal{O}\|$.

We refer the readers to the full version of this paper [26, Appendix B] for the proof of this lemma.

[3] For a precise definition of an index sequence, see Definition 4 of [21].

3 Simulating open quantum systems with time-dependent Lindbladian

Ref. [36, Section 6] sketched a method for simulating open quantum systems with time-dependent Lindbladian. In this section, we present the details of this simulation algorithm.

Motivated by the time scaling idea in [5], we define a change-of-variable function as

$$\mathrm{var}(t) \coloneqq \int_0^t \mathrm{d}s \, \|\mathcal{L}(s)\|_{\mathrm{be}}. \tag{16}$$

By simulating the Lindblad dynamics on the new time scale, the overall complexity exhibits a better dependence on the norm of the Lindbladians in time. To this end, we need the following oracle to perform the inverse change-of-variable:

$$\mathcal{O}_{\mathrm{var}} |t\rangle |z\rangle = |t\rangle \left|z \oplus \mathrm{var}^{-1}(t)\right\rangle. \tag{17}$$

In addition, we need the following oracle to obtain the normalizing constant $\alpha_0(t)$ for $H(t)$ and $\alpha_j(t)$ for $L_j(t)$: for all $j = [m]$,

$$\mathcal{O}_{H,\mathrm{norm}} |t\rangle |z\rangle = |t\rangle |z \oplus \alpha_0(t)\rangle, \quad \text{and} \quad \mathcal{O}_{L_j,\mathrm{norm}} |t\rangle |z\rangle = |t\rangle |z \oplus \alpha_j(t)\rangle. \tag{18}$$

As in [36], we define the *block-encoding norm* for a Lindbladian $\mathcal{L}$, denoted by $\|\mathcal{L}\|_{\mathrm{be}}$ for normalization purposed:

$$\|\mathcal{L}\|_{\mathrm{be}} \coloneqq \alpha_0 + \frac{1}{2}\sum_{j=1}^{m} \alpha_j^2. \tag{19}$$

The goal of this section is to prove the following theorem.

▶ **Theorem 11.** *Suppose we are given an $(\alpha_0(t), a, \epsilon')$-block-encoding $U_{H(t)}$ of $H(t)$, and an $(\alpha_j(t), a, \epsilon')$-block-encoding $U_{L_j(t)}$ for each $L_j(t)$ for all $0 \le t \le T$. Let $\|\mathcal{L}\|_{\mathrm{be},1}$ be defined as $\|\mathcal{L}\|_{\mathrm{be},1} \coloneqq \int_0^T \mathrm{d}\tau \, \|\mathcal{L}(\tau)\|_{\mathrm{be}}$, Suppose further that $\epsilon' \le \epsilon/(2t(m+1))$. Then, there exists a quantum algorithm that outputs a purification of $\tilde{\rho}_T$ of $\tilde{\rho}(T)$ where $\left\| \tilde{\rho}(T) - \mathcal{T} e^{\int_0^T \mathrm{d}\tau \, \mathcal{L}(\tau)}(\rho_0) \right\|_1 \le \epsilon$ using*

$$O\left(\|\mathcal{L}\|_{\mathrm{be},1} \left(\frac{\log\left(\|\mathcal{L}\|_{\mathrm{be},1}/\epsilon\right)}{\log\log\left(\|\mathcal{L}\|_{\mathrm{be},1}/\epsilon\right)} \right)^2 \right) \tag{20}$$

queries to $U_{H(t)}$, $U_{L_j(t)}$, $\mathcal{O}_{\mathrm{var}}$, $\mathcal{O}_{H,\mathrm{norm}}$, and $\mathcal{O}_{L_j,\mathrm{norm}}$, and $\widetilde{O}\left((m+n)\|\mathcal{L}\|_{\mathrm{be},1}\right)$ additional 1- and 2-qubit gates, where n is the number of qubits the Lindbladian is acting on.

3.1 High-level overview of the simulation algorithm

Here we briefly outline the techniques that led to the stated complexity. Let the Hamiltonian $H(t) = H_0 + \sum_\beta u_\beta(t)\mu_\beta$, we rewrite equation (1) as follows

$$\frac{d}{dt}\rho = \mathcal{L}(t)(\rho) \coloneqq -i[H(t), \rho] + \sum_{j=1}^{m} (L_j(t)\rho L_j^\dagger(t) - \frac{1}{2}\{L_j(t)^\dagger L_j(t), \rho\}) \tag{21}$$

$$= \mathcal{L}_D(t)(\rho) + \mathcal{L}_J(t)(\rho). \tag{22}$$

Here we have decomposed the Lindbladian into a drift term $\mathcal{L}_{\mathrm{D}}(t)$ and a jump term $\mathcal{L}_{\mathrm{J}}(t)$:

$$\mathcal{L}_{\mathrm{D}}(t)(\rho) = -i[H(t),\rho] - \frac{1}{2}\sum_{j=1}^{m}\{L_j(t)^\dagger L_j(t),\rho\} = J(t)\rho + \rho J(t)^\dagger, \tag{23}$$

$$\mathcal{L}_{\mathrm{J}}(t)(\rho) = \sum_{j=1}^{m} L_j(t)\rho L_j(t)^\dagger, \tag{24}$$

where $J(t) \coloneqq -iH(t) - \frac{1}{2}\sum_{j=1}^{m} L_j(t)^\dagger L_j(t)$.

With the known initial value $\rho(0) = \rho_0$, the solution of Eq. (22) can be written as the linear combination of the following equations.

$$\begin{cases} \partial_t \rho &= \mathcal{L}_{\mathrm{D}}(t)(\rho) \\ \rho(0) &= \rho_0 \end{cases}, \quad \text{and} \quad \begin{cases} \partial_t \rho &= \mathcal{L}_{\mathrm{D}}(t)(\rho) + \mathcal{L}_{\mathrm{J}}(t)(\rho) \\ \rho(0) &= 0 \end{cases}. \tag{25}$$

Specifically, for the first part of Eq. (25), the density operator follows $\rho(t) = V(0,t)\rho_0 V(0,t)^\dagger = \mathcal{K}[V(0,t)](\rho_0)$, where $V(s,t) = \mathcal{T}e^{\int_s^t J(\tau)\mathrm{d}\tau}$ is the time-ordered exponential of J. A brief introduction of time-ordered exponential can be found in in the full version of this paper ([26, Appendix A]). For the second part of Eq. (25), the density operator follows $\rho(t) = \int_0^t g(t,s)\mathrm{d}s$, where the function $g(t,s)$ satisfying

$$\partial_t g(t,s) = \mathcal{L}_{\mathrm{D}}(t)(g(t,s)), \text{ and } \lim_{t\to s} g(t,s) = \mathcal{L}_{\mathrm{J}}(s)(\rho(s)). \tag{26}$$

By using time-ordered evolution operator and Duhamel's principle, the solution of Eq. (21) can be expressed as

$$\rho(t) = \mathcal{K}[V(0,t)](\rho_0) + \int_0^t \mathcal{K}[V(s,t)](\mathcal{L}_{\mathrm{J}}(s)(\rho(s)))\,\mathrm{d}s. \tag{27}$$

The time-ordered exponential $V(0,t)$ can be approximated by the truncated Dyson series (see the full version of this paper [26, Appendix A.1] for details),

$$V(0,t) = \mathcal{T}e^{\int_0^t J(\tau)\mathrm{d}\tau} \approx \sum_{k=0}^{K}\frac{1}{k!}\mathcal{T}\int_0^t \mathrm{d}\boldsymbol{\tau} J(\tau_k)\cdots J(\tau_1), \tag{28}$$

where $\mathcal{T}\int_0^t \mathrm{d}\boldsymbol{\tau}(\cdot)$ denote an integration over a k-tuple of time variables $(\tau_1,\ldots,\tau_k)$ while keeping the time ordering: $\tau_1 \le \tau_2 \le \cdots \le \tau_k$. Thus,

$$V(s,t) = \mathcal{T}e^{\int_s^t J(\tau)\mathrm{d}\tau} = \mathcal{T}e^{\int_0^{t-s} J(s+\tau)\mathrm{d}\tau} \tag{29}$$

$$\approx \sum_{k=0}^{K}\frac{1}{k!}\int_0^{t-s} \mathrm{d}\boldsymbol{\tau}\mathcal{T}[J(\tau_k)\cdots J(\tau_1)]. \tag{30}$$

As in [30], we use the rectangle rule to approximate the integral in the truncated Dyson series. Note that more efficient quadratures could be potentially used as we use later approximation the integral in Eq. (27), for instance, the scaled Gaussian quadrature; however such methods require upper bounds on higher-order derivatives of $J(t)$, which are not readily available.

By applying Duhamel's principle (see Eq. (27)) several times, we obtain the following approximation with notations introduced in [10].

$$\mathcal{G}_K(t) \coloneqq \mathcal{K}[V(0,t)] + \sum_{k=1}^{K}\int_{0\le s_1\le\cdots\le s_k\le t} \mathcal{F}_k(s_k,\ldots,s_1)\,\mathrm{d}s_1\cdots\mathrm{d}s_k, \tag{31}$$

where

$$\mathcal{F}_k(s_k,\dots,s_1) \coloneqq \mathcal{K}[V(s_k,t)]\mathcal{L}_{\mathrm{J}}(s_k)\cdots\mathcal{K}[V(s_1,s_2)]\mathcal{L}_{\mathrm{J}}(s_1)\mathcal{K}[V(0,s_1)]. \tag{32}$$

This yields an approximation of the evolution superoperator $\rho(t) \approx \mathcal{G}_K(t)(\rho(0))$. The key observation is that $\mathcal{F}_k$ is a composition of CPTP maps. The second term of $\mathcal{G}_K(t)$ can be approximated by using truncated Dyson series.

3.2 Detailed constructions

In this subsection, we present the construction of the time-dependent Lindbladian simulation algorithm. For the sake of conciseness, we omit the convoluted details in treating the time-ordering of the truncated Dyson series. All these details can be found in the full version of this paper [26, Appendix D].

The scaled evolution time

Recall that we introduced the rescaled time in Eq. (16), and let define $\hat{t}$ as

$$\hat{t} = \mathrm{var}(t) = \int_0^t \mathrm{d}s \, \|\mathcal{L}(s)\|_{\mathrm{be}}. \tag{33}$$

Correspondingly, we follow the rescaled Lindblad equation, by defining $\hat{\rho}(\hat{t}) = \rho((\mathrm{var}^{-1}(\hat{t}))$, which, from Eq. (1), satisfies the equation

$$\frac{\mathrm{d}}{\mathrm{d}\hat{t}}\hat{\rho}(\hat{t}) = \widehat{\mathcal{L}}(\hat{t})\hat{\rho}(\hat{t}), \tag{34}$$

where the rescaled Lindbladian is as,

$$\widehat{\mathcal{L}}(\hat{t}) = \frac{\mathcal{L}(\mathrm{var}^{-1}(\hat{t}))}{\left\|\mathcal{L}(\mathrm{var}^{-1}(\hat{t}))\right\|_{\mathrm{be}}}. \tag{35}$$

This rescaling can be achieved by defining

$$\widehat{H}(\hat{t}) \coloneqq \frac{H(\mathrm{var}^{-1}(\hat{t}))}{\left\|\mathcal{L}(\mathrm{var}^{-1}(\hat{t}))\right\|_{\mathrm{be}}}, \text{ and } \widehat{L}(\hat{t}) \coloneqq \frac{L(\mathrm{var}^{-1}(\hat{t}))}{\sqrt{\left\|\mathcal{L}(\mathrm{var}^{-1}(\hat{t}))\right\|_{\mathrm{be}}}}. \tag{36}$$

The *scaled effective Hamiltonian* (not Hermitian), denoted by $\widehat{J}(\hat{t})$, is therefore defined as

$$\widehat{J}(\hat{t}) \coloneqq \frac{J(\mathrm{var}^{-1}(\hat{t}))}{\left\|\mathcal{L}(\mathrm{var}^{-1}(\hat{t}))\right\|_{\mathrm{be}}}. \tag{37}$$

As a result, simulating $\widehat{\mathcal{L}}$ for time $\hat{t} = \mathrm{var}(t)$ is equivalent to simulating $\mathcal{L}$ for time t. Moreover, the block-encoding-norm of $\widehat{\mathcal{L}}$ is at most 1 because of Eq. (35).

To simplify the notation, in the remainder of this section we assume the Lindbladian is already scaled so that we can drop the $\widehat{\cdot}$ notation for the scaled operators and evolution time.

LCU construction

Let $U_J(t)$ be an (α, a, ϵ)-block-encoding of $J(t)$. Given the oracles as in Eqs. (4) and (5), the unitary $\sum_t |t\rangle\langle t| \otimes U_J(t)$ for discretized times t can be implemented. Using Lemma 3, a block-encoding of $V(s,t)$ can also be implemented. More specifically, we use the rectangle rule as in [30] to approximate the integrals in Eq. (30):

$$\widetilde{V}(s,t) = \sum_{k=0}^{K'} \frac{(t-s)^k}{M^k k!} \sum_{j_1,\dots,j_k=0}^{M-1} \mathcal{T} J(t_{j_k})\cdots J(t_{j_1}). \tag{38}$$

Here the time-ordered term is defined as follows, for each tuple $t_k, t_{k-1}, \ldots, t_1$,

$$\mathcal{T}J(t_k)\cdots J(t_1) = J(t_{j_k})\cdots J(t_{j_1}),$$

where $t_{j_k}, \ldots, t_{j_1}$ is the permutation of $t_k, t_{k-1}, \ldots, t_1$ that is in ascending order.

The error of the above approximation is bounded by

$$\left\| V(s,t) - \widetilde{V}(s,t) \right\| \leq O\left(\frac{(t-s)^{K'+1}}{(K'+1)!} + \frac{(t-s)^2 \dot{J}_{\max}}{M} \right), \tag{39}$$

where $\dot{J}_{\max} \coloneqq \max_{\tau\in[0,t]} \left\| \frac{\mathrm{d}J(\tau)}{\mathrm{d}\tau} \right\|$.

Now, we need to approximate the integrals in Eq. (31). In [36], Gaussian quadratures were used to approximate similar integrals in the time-independent case, which yields a simpler LCU construction. Unfortunately, using such efficient quadrature rules in the time-dependent case requires bounding the norm of high-order derivatives of $V(s,t)$, which is not directly given. Instead, we use the simple Riemann sums for treating the integrals, where the LCU constructions follow closely from the ones in [30].

More specifically, we uniformly divide the evolution time t into q intervals, and let $t_j = tj/q$ for $j \in \{0, \ldots, M-1\}$. Assuming $V(s,t)$ is implemented perfectly, we consider the following superoperator,

$$\frac{t^k}{k!q^k} \sum_{j_1,\ldots,j_k=0}^{q} \mathcal{T}\mathcal{F}_k(t_{j_k}, \ldots, t_{j_1}), \tag{40}$$

which approximates the integrals in Eq. (31). To bound the quality of this approximation, we need to bound the derivative of $\mathcal{F}_k$. We begin by bounding $\|V(0,t)\|$, which can be deduced from the stability of the differential equation $\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{y} = J(t)\boldsymbol{y}$, which can be studied by examining the eigenvalues of the Hermitian part of $J(t)$ [7, Lemma 1]. Since the Hermitian part of $J(t)$ is semi-negative definite, one has $\|\boldsymbol{y}(t)\| \leq \|\boldsymbol{y}(0)\|$, which implies that

$$\|V(0,t)\| \leq 1. \tag{41}$$

Since $\frac{\mathrm{d}}{\mathrm{d}t}V(0,t) = J(t)V(0,t)$, the derivative of $V(0,t)$ can be bounded by

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t}V(0,t) \right\| \leq \dot{J}_{\max}. \tag{42}$$

We further consider $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}[V(0,t)]$. For any operator A with $\|A\|_1 = 1$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}[V(0,t)](A) = \left(\frac{\mathrm{d}}{\mathrm{d}t}V(0,t)\right) AV(0,t)^\dagger + V(0,t)A\frac{\mathrm{d}}{\mathrm{d}t}V(0,t)^\dagger. \tag{43}$$

We then have $\left\| \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}[V(0,t)](A) \right\|_1 \leq 2\dot{J}_{\max}$, which follows from Eqs. (41) and (42) and the fact that $\|BAC\|_1 \leq \|B\|\|A\|_1\|C\|$ for matrices A, B, C. This bound easily extends to the diamond norm by tensoring the Kraus operator with an identity operator to extend it to a larger space. Hence, we have

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}[V(0,t)](A) \right\|_\diamond \leq 2\dot{J}_{\max}. \tag{44}$$

Let $\dot{L}_{j,\max}$ be defined as $\dot{L}_{j,\max} \coloneqq \max_{\tau\in[0,t]} \left\| \frac{\mathrm{d}}{\mathrm{d}\tau}L_j(\tau) \right\|$. Then, using similar arguments, we can bound the derivative of $\mathcal{L}_\mathrm{J}(t)$ as

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{L}_\mathrm{J}(t) \right\|_\diamond \leq 2\sum_{j=1}^{m} \dot{L}_{j,\max}, \tag{45}$$

where we have assumed that the Lindbladian is scaled as in Eq. (35), i.e., $\|L_j\| \leq 1$. For the derivative of $\mathcal{F}_k$, we have

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t_j}\mathcal{F}_k \\
&= \mathcal{K}[V(t_k,t)]\mathcal{L}_{\mathrm{J}}(t_k)\cdots\frac{\mathrm{d}}{\mathrm{d}t_j}\left(\mathcal{K}[V(t_j,t_{j+1})]\mathcal{L}_{\mathrm{J}}(t_j)\mathcal{K}[V(t_{j-1},t_j)]\right)\mathcal{L}_{\mathrm{J}}(t_{j-1})\cdots\mathcal{K}[V(0,t_1)] \\
&= \mathcal{K}[V(t_k,t)]\mathcal{L}_{\mathrm{J}}(t_k)\cdots\frac{\mathrm{d}}{\mathrm{d}t_j}(\mathcal{K}[V(t_j,t_{j+1})])\mathcal{L}_{\mathrm{J}}(t_j)\mathcal{K}[V(t_{j-1},t_j)]\mathcal{L}_{\mathrm{J}}(t_{j-1})\cdots\mathcal{K}[V(0,t_1)] \quad (46)\\
&+ \mathcal{K}[V(t_k,t)]\mathcal{L}_{\mathrm{J}}(t_k)\cdots\mathcal{K}[V(t_j,t_{j+1})]\frac{\mathrm{d}}{\mathrm{d}t_j}(\mathcal{L}_{\mathrm{J}}(t_j))\mathcal{K}[V(t_{j-1},t_j)]\mathcal{L}_{\mathrm{J}}(t_{j-1})\cdots\mathcal{K}[V(0,t_1)] \\
&+ \mathcal{K}[V(t_k,t)]\mathcal{L}_{\mathrm{J}}(t_k)\cdots\mathcal{K}[V(t_j,t_{j+1})]\mathcal{L}_{\mathrm{J}}(t_j)\frac{\mathrm{d}}{\mathrm{d}t_j}(\mathcal{K}[V(t_{j-1},t_j)])\mathcal{L}_{\mathrm{J}}(t_{j-1})\cdots\mathcal{K}[V(0,t_1)].
\end{aligned}$$

Again, assume the Lindbladian is scaled as in Eq. (35), the above expression of $\frac{\mathrm{d}}{\mathrm{d}t_j}\mathcal{F}_k$ together with Eqs. (44) and (45) implies that $\left\|\frac{\mathrm{d}}{\mathrm{d}t_j}\mathcal{F}_k\right\|_\diamond \leq 4\dot{J}_{\max} + 2\sum_{j=1}^m \dot{L}_{j,\max}$. This implies that the error for using the Riemann sums can be bounded by

$$\begin{aligned}
&\left\|\mathcal{G}_K - \mathcal{K}[V(0,t)] - \frac{t^k}{k!q^k}\sum_{k=1}^K\sum_{j_1,\ldots,j_k=0}^q \mathcal{T}\mathcal{F}_k(t_{j_k},\ldots,t_{j_1})\right\|_\diamond \\
&= \left\|\sum_{k=1}^K\int_{0\leq s_1\leq\cdots\leq s_k\leq t}\mathcal{F}_k(s_k,\ldots,s_1)\,\mathrm{d}s_1\cdots\mathrm{d}s_k - \frac{t^k}{k!q^k}\sum_{k=1}^K\sum_{j_1,\ldots,j_k=0}^q \mathcal{T}\mathcal{F}_k(t_{j_k},\ldots,t_{j_1})\right\|_\diamond \\
&\leq \sum_{k=1}^K\frac{t^2}{q}\cdot\left(4\dot{J}_{\max} + 2\sum_{j=1}^m\dot{L}_{j,\max}\right) \quad (47)\\
&= \frac{Kt^2}{q}\cdot\left(4\dot{J}_{\max} + 2\sum_{j=1}^m\dot{L}_{j,\max}\right). \quad (48)
\end{aligned}$$

In addition, it is easy to see that the error caused by using Duhamel's principle is

$$\left\|e^{\mathcal{T}\int_0^t \mathrm{d}\tau\,\mathcal{L}(\tau)} - \mathcal{G}_K\right\|_\diamond \leq \frac{(2t)^{K+1}}{(K+1)!}. \quad (49)$$

It follows from Eqs. (48) and (49) that

$$\begin{aligned}
&\left\|e^{\mathcal{T}\int_0^t \mathrm{d}\tau\,\mathcal{L}(\tau)} - \mathcal{K}[V(0,t)] - \frac{t^k}{k!q^k}\sum_{j_1,\ldots,j_k=0}^q \mathcal{T}\mathcal{F}_k(t_{j_k},\ldots,t_{j_1})\right\|_\diamond \\
&\leq \frac{(2t)^{K+1}}{(K+1)!} + \frac{Kt^2}{q}\left(4\dot{J}_{\max} + 2\sum_{j=1}^m\dot{L}_{j,\max}\right).
\end{aligned} \quad (50)$$

Finally, we have the following LCU form:

$$\widetilde{\mathcal{G}}_K \coloneqq \mathcal{K}[\widetilde{V}(0,t)] + \sum_{k=1}^K\frac{t^k}{q^k}\sum_{j_1,\ldots,j_k=0}^q \widetilde{\mathcal{F}}_k(t_{j_k},\ldots,t_{j_1}), \quad (51)$$

where $\widetilde{\mathcal{F}}_K$ is an approximation of Eq. (32) by using $\widetilde{V}(s,t)$ instead of $V(s,t)$, i.e.,

$$\widetilde{\mathcal{F}}_k(s_k,\ldots,s_1) \coloneqq \mathcal{K}[\widetilde{V}(s_k,t)]\mathcal{L}_J(s_k)\mathcal{K}[\widetilde{V}(s_{k-1},s_k)]\cdots\mathcal{K}[\widetilde{V}(s_1,s_2)]\mathcal{L}_J(s_1)\mathcal{K}[\widetilde{V}(0,s_1)]. \quad (52)$$

We use the same compression scheme as in [30] to deal with the time-ordering in Eqs. (38) and (51). Note that implementing the LCU requires additional $O(KK'm(\log M + \log q + n))$ 1- and 2-qubit gates.

Complexity analysis

We first analyze the normalizing constant for the LCU implementation. Recall that we are working with scaled operators, so the normalizing factors are at most 1. For the implement of $V(0,\hat{t})$, we can use, for example, the LCU construction involving quantum sort as in [30] for implement Eq. (38). If we further assume the implementation uses an infinite Dyson series, the normalizing constants of the block-encoding $\mathcal{K}[V(0,t)]$ is upper bounded by

$$\sum_{k=0}^{\infty}\frac{t^k}{k!} = e^t. \quad (53)$$

As a result, the sum-of-squares of the normalizing constants of the Kraus operators of $\mathcal{F}_k(\hat{t}_k,\ldots,\hat{t}_1)$ can be bounded by

$$\sum_{j_1,\ldots,j_k=0}^{m} e^{2(t-s_k)}e^{2(s_k-s_{k-1})}\ldots e^{2(s_1-0)} = e^{2t}. \quad (54)$$

Recall that the normalizing constant for L_j is 1 since the Lindbladian is rescaled. For the second term in Eq. (31), the sum-of-squares of the normalizing constants of the Kraus operators can be bounded by

$$e^{2t}\frac{t^k}{k!q^k}q^k = e^{2t}\frac{t^k}{k!}. \quad (55)$$

By Eqs. (53) and (55), we have that the sum-of-squares of the normalizing constants of the Kraus operators of the LCU in Eq. (31) can then be bounded by $e^{2t}+\sum_{k=1}^{K}e^{2t}\frac{t^k}{k!} \le e^{2t}+e^{3t}$.

Therefore, it suffices to set $t=\Omega(1)$ to achieve constant success probability when using Lemma 2. Then, we use the oblivious amplitude amplification for channels [15] to boost the success probability to 1 with constant applications of Lemma 2. For the error bound in Eq. (50), assume for now that the second error term is dominated by the first (by some choice of q to be determined). It suffices to set $K=\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}$ to make the total error at most $\epsilon/2$, because of the choice of $t=\Omega(1)$. The choice of q satisfies

$$q = \Theta\left(\frac{2K}{\epsilon}\left(4\dot{J}_{\max}+2\sum_{j=1}^{m}\dot{L}_{j,\max}\right)\right). \quad (56)$$

Now, we deal with the error from truncated Dyson series and Riemann sum to implement $V(s,t)$. By Eq. (38), we can choose M large enough (determined later) so that the second error term is dominated by the first. Then, using [36, Lemma 7], we have

$$\left\|\mathcal{F}_k(s_k,\ldots,s_1)-\widetilde{\mathcal{F}}_k(s_k,\ldots,s_1)\right\|_{\diamond} \le \frac{8e^t}{(K'+1)!}2^{k+1}t^{K'+1}. \quad (57)$$

Further, using the analysis as in [36], we can bound the total approximation error (with appropriate choice of M to be determined later) as

$$\left\| \mathcal{T} e^{\int_0^t \mathcal{L}(\tau) \mathrm{d}\boldsymbol{\tau}} - \widetilde{\mathcal{G}}_K \right\|_\diamond \leq \frac{32 e^{5t} t^{K'+2}}{(K'+1)!}. \tag{58}$$

With the choice of $t = \Omega(1)$, we can choose $K' = \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}$ so that the total error is bounded by ϵ. For the choice of M, we need to make sure the second error term in Eq. (38) is dominated by the first term. Hence we can choose $M = \Theta\left(\frac{j_{\max}}{\epsilon}\right)$.

It remains to analyze the cost for the LCU implementation, which is the same as the analyses in [36] and [30]. Note that the dependence on M is logarithmic if the compressed scheme is used in [30] for implementing $\widetilde{V}(s,t)$. The total gate cost is now upper bounded by $O(KK'm(\log M + \log q + n))$. Further note that the error ϵ' brought by the block-encoding can be eventually transferred to $\mathcal{L}$ causing an $(m+1)\epsilon'$ error on $\mathcal{L}$ in terms of the diamond norm, and the accumulated error for evolution time t is then at most $t(m+1)\epsilon'$. As a result, choosing $\epsilon' \leq \epsilon/(2t(m+1))$ suffices to ensure the total error is at most ϵ.

Recall that the above analysis is based on the scaled version of $\mathcal{L}$ defined in Eq. (35), and the evolution time is scaled as in Eq. (33). For arbitrary evolution time $\hat{t}$, we apply the above procedure $O(\hat{t})$ times with precision $\epsilon' = \epsilon/\hat{t}$. This gives the desired complexity in Theorem 11. Lastly, it is important to note that the LCU circuit yields a purification of $\rho(t)$. This completes the proof of Theorem 11.

Note that the above analysis easily extends to the simulation of the original Lindbladian without any scaling, where the complexity depends linearly on the product of evolution time and the maximum of the block-encoding norm of the Lindbladian. More specifically, we have the following corollary.

▶ **Corollary 12.** *Suppose we are given an $(\alpha_0(t), a, \epsilon')$-block-encoding $U_{H(t)}$ of $H(t)$, and an $(\alpha_j(t), a, \epsilon')$-block-encoding $U_{L_j(t)}$ for each $L_j(t)$ for all $t \geq 0$. Define $\|\mathcal{L}\|_{\mathrm{be},\infty}$ as $\|\mathcal{L}\|_{\mathrm{be},\infty} \coloneqq \max_{\tau\in[0,T]} \|\mathcal{L}(\tau)\|_{\mathrm{be}}$. Suppose further that $\epsilon' \leq \epsilon/(2T(m+1))$. There exists a quantum algorithm that outputs a purification of $\tilde{\rho}(T)$ where $\|\tilde{\rho}(T) - e^{\mathcal{T}\int_0^T \mathrm{d}\tau\, \mathcal{L}(\tau)}(\rho_0)\|_1 \leq \epsilon$ using*

$$O\left(T\|\mathcal{L}\|_{\mathrm{be},\infty} \left(\frac{\log\left(T\|\mathcal{L}\|_{\mathrm{be},\infty}/\epsilon\right)}{\log\log\left(T\|\mathcal{L}\|_{\mathrm{be},\infty}/\epsilon\right)} \right)^2 \right) \tag{59}$$

queries to $U_{H(t)}$, $U_{L_j(t)}$, $\mathcal{O}_{\mathrm{var}}$, $\mathcal{O}_{H,\mathrm{norm}}$, and $\mathcal{O}_{L_j,\mathrm{norm}}$, and $\widetilde{O}\left((m+n)T\|\mathcal{L}\|_{\mathrm{be},\infty}\right)$ additional 1- and 2-qubit gates. Here, n is the number of qubits the Lindbladian is acting on.

4 Simulations in the Interaction Picture

Many control problems involve a system Hamiltonian that contains a time-independent Hamiltonian that dominates the spectral norm $H(t)$, and thus the overall computational complexity. Motivated by the interaction picture approach for Hamiltonian simulations [41], we devise an approach to simulate the Lindblad dynamics. To formulate the problem, we assume that the Lindbladian admits the following decomposition:

$$\mathcal{L}(\cdot) = -i\left[H_1 + H_2(t), \cdot\right] + \sum_j L_j(\cdot)L_j^\dagger - \frac{1}{2}\left\{L_j^\dagger L_j, \cdot\right\}, \tag{60}$$

where H_1 is a time-independent free Hamiltonian, $H_2(t)$ is the coupling Hamiltonian which contains the control variables, and the dissipative terms still come from the interaction with the environment.

One such example is the control of an ion trap system [25], in which the model Hamiltonian consists of the following terms,

$$H_1 = \hbar \sum_{i=1}^{N} \left(\omega_{01} |1\rangle_i \langle 1| + \omega_{0e} |e\rangle_i \langle e|\right) + \hbar \sum_k \omega_k a_k^\dagger a_k \tag{61}$$

$$H_2(t) = \hbar\Omega_1 \cos\left(\boldsymbol{k}_1 \cdot \boldsymbol{r}_j - \omega_1 t - \varphi_1\right) \left(|0\rangle_j\langle e| + |e\rangle_j\langle 0|\right) \tag{62}$$

$$+ \hbar\Omega_2 \cos\left(\boldsymbol{k}_2 \cdot \boldsymbol{r}_j - \omega_2 t - \varphi_2\right) \left(|1\rangle_j\langle e| + |e\rangle_j\langle 1|\right), \tag{63}$$

and L_js includes $\lambda_{\text{heat}} a_j^\dagger$, $\lambda_{\text{damp}} a_j$ and $\lambda_{\text{dephase}} n_j$. The observation in [25] is that $\omega_{0e} \gg |\Omega_1|, |\Omega_2| \gg \lambda_{\text{heat}}, \lambda_{\text{damp}}, \lambda_{\text{dephase}}$.

Motivated by such applications, we assume that in Eq. (60),

$$\|H_1\| \gg \|H_2(t)\| \gg \|L_j\|. \tag{64}$$

In the interaction approach, e.g., [41], one simulates the density operator in the interaction picture, where the large magnitude of H_1 is absorbed into the slow Hamiltonian $H_2(t)$ and the jump operators. In this section, we provide detailed quantum algorithms for simulating the Lindbladian Eq. (60) in the interaction picture.

4.1 Lindbladian simulation in interaction picture

In light of Eq. (60), we first write the Lindbladian into two parts

$$\mathcal{L}(t) = \mathcal{L}_1 + \mathcal{L}_2(t) \tag{65}$$

where $\mathcal{L}_1$ contains a time-independent Hamiltonian term and $\mathcal{L}_2(t)$ can be a general Lindbladian term

$$\mathcal{L}_1(\cdot) = -i\left[H_1, \cdot\right] \tag{66}$$

$$\mathcal{L}_2(t)(\cdot) = -i\left[H_2(t), \cdot\right] + \sum_j L_j(\cdot)L_j^\dagger - \left\{L_j^\dagger L_j, \cdot\right\}. \tag{67}$$

Then the Lindblad master equation in Eq. (1) is equivalent to:

$$\frac{\mathrm{d}}{\mathrm{d}t} V_1\dagger(t_0,t)\rho V_1(t_0,t) = V_1^\dagger(t_0,t)\mathcal{L}_2(t)V_1(t_0,t)V_1^\dagger(t_0,t)\rho V_1(t_0,t), \tag{68}$$

where $V_1(t_0,t) = e^{-iH_1(t-t_0)}$, and $t \geq t_0$.

We can define $\rho_{\text{I}} = V_1^\dagger(t_0,t)\rho V_1(t_0,t)$ as the density operator in the interaction picture, and it satisfies the Lindblad equation, $\frac{d}{dt}\rho_{\text{I}}(t) = \mathcal{L}_{2,\text{I}}(t)\rho_{\text{I}}(t)$, where $\mathcal{L}_{2,\text{I}}(t) \coloneqq V_1^\dagger(t_0,t)\mathcal{L}_2(t)V_1(t_0,t)$. Effectively, this transforms H_2 and $L_j(t)$ in Eq. (67) into an interaction picture as well.

By simulating the time evolution in the interaction picture and transforming it back to the original picture at last, we have

$$\rho(t) = \left(e^{\mathcal{L}_1(t-t_0)}\right)\left(\mathcal{T}e^{\int_{t_0}^{t}\mathcal{L}_{2,\text{I}}(s)\mathrm{d}s}\rho(t_0)\right), \tag{69}$$

where $\left(e^{\mathcal{L}_1(b-a)}\right)(\cdot) = V_1(a,b)(\cdot)V_1^{-1}(a,b)$. We can further decompose this evolution into N Trotter steps (with $\tau = (t-t_0)/N$),

$$\rho(t) = \prod_{i=0}^{N-1}\left(e^{\mathcal{L}_1\tau}\mathcal{T}e^{\int_{t_0+i\tau}^{t_0+(i+1)\tau}\mathcal{L}_{2,\mathrm{I}}(s)\mathrm{d}s}\right)\rho(t_0). \tag{70}$$

At a high level, Eq. (70) summarizes our simulation strategy in the interaction picture. The total time complexity is determined by the number of time steps N, and the time complexity in each step, which follows from our Lindbladian simulation algorithm in Section 3.

▶ **Theorem 13** (Modified from Corollary 12). *Suppose we are given an (α_0, a, ϵ')-block-encoding U_H of H, and an (α_j, a, ϵ')-block-encoding U_{L_j} for each L_j. For all $\tau, \epsilon' \geq 0$ and $t\|\mathcal{L}(\tau)\|_{\mathrm{be},\infty} = \Theta(1)$, there exists a quantum algorithm for simulating $e^{\mathcal{L}\tau}$ using $O\big(\frac{\log(1/\epsilon')}{\log\log(1/\epsilon')}\big)$ queries to U_H and U_{L_j} and $O\big(m\big(\frac{\log(1/\epsilon')}{\log\log(1/\epsilon')}\big)^2\big)$ additional 1- and 2-qubit gates.*

▶ **Lemma 14** (Error accumulation). *Given that $A_j = W_j$ and $B_j = \mathcal{T}\left[e^{\int_{t_{j-1}}^{t_j}\mathcal{L}_1(s)\mathrm{d}s}\right]$ are bounded $\|W_j\| \leq 1$, $\|B_j\| \leq 1$, and error in each segment is bounded by δ $\|A_j - B_j\| \leq \delta$. Then the accumulated error is*

$$\left\|\prod_j^L W_j - \mathcal{T}\left[e^{\int_0^t \mathcal{L}(s)\mathrm{d}s}\right]\right\| \leq L\delta. \tag{71}$$

Proof. The lemma holds by applying the triangle inequality

$$\left\|\prod_{j=1}^L A_j - \prod_{j=1}^L B_j\right\| \leq \sum_{k=1}^L \left(\prod_{j=1}^{k-1}\|A_j\|\right)\|A_k - B_k\|\left(\prod_{j=k+1}^L \|B_j\|\right). \tag{72}$$

◀

These results imply the following result for Lindbladian simulation in the interaction picture:

▶ **Theorem 15** (Query complexity of Lindbladian simulation in the interaction picture). *Let $\mathcal{L}(t) = \mathcal{L}_1(t) + \mathcal{L}_2(t)$, with $\mathcal{L}_1(t)$ and $\mathcal{L}_2(t)$ defined by Eqs. (66) and (67) respectively. Assume the existence of a unitary oracle that implements the Hamiltonian and Lindbladian within the interaction picture, denoted U_{H^I} and $U_{L_j^I}$ which implicitly depends on the time-step size $\tau \in \mathcal{O}\left(||\mathcal{L}_2||_{\mathrm{be}}^{-1}\right)$ and number of quadrature points q, such that*

$$\left(\langle 0|_a \otimes \mathbf{1}_s\right) U_{H^I}\left(|0\rangle_a \otimes \mathbf{1}_s\right) = \sum_{j_k=1}^q |j_k\rangle\langle j_k| \otimes \frac{e^{iH_1\tau\hat{x}_{(j_k)}} H_2 e^{-iH_1\tau\hat{x}_{(j_k)}}}{\alpha_H} \tag{73}$$

$$\left(\langle 0|_a \otimes \mathbf{1}_s\right) U_{L_j^I}\left(|0\rangle_a \otimes \mathbf{1}_s\right) = \sum_{j_k=1}^q |j_k\rangle\langle j_k| \otimes \frac{e^{iH_1\tau\hat{x}_{(j_k)}} L_j e^{-iH_1\tau\hat{x}_{(j_k)}}}{\alpha_{L_j}}, \tag{74}$$

For $t \geq ||\mathcal{L}_2(t)||_{\mathrm{be}}\tau$, the time-evolution operator $\mathcal{T}e^{\int_0^t \mathcal{L}_1(s)+\mathcal{L}_2(s)\mathrm{d}s}$ may be approximated to error ϵ with the following cost.

1. *Simulations of $e^{-iH_1\tau}$: $\mathcal{O}\left(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}\right)$,*
2. *Queries to U_{H^I} and $U_{L_j^I}$: $\mathcal{O}\left(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}\frac{\log(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}/\epsilon)}{\log\log(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}/\epsilon)}\right)$,*
3. *Primitive gates: $\mathcal{O}\left(mt||\mathcal{L}_2(t)||_{\mathrm{be},\infty}(\frac{\log(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}/\epsilon)}{\log\log(t||\mathcal{L}_2(t)||_{\mathrm{be},\infty}/\epsilon)})^2\right)$.*

Proof. Consider simulation strategy shown in Eq. (70), we uniformly divide the evolution time $[0,t]$ into $M = \lceil t \left\|\mathcal{L}_2(t)\right\|_{\mathrm{be},\infty} \rceil$, time step $\tau = t/M$. Then $\tau \left\|\mathcal{L}_2(t)\right\|_{\mathrm{be},\infty} = \Theta(1)$, which satisfies the pre-condition of Theorem 13. Therefore, using Theorem 13, the time and gate complexity of each time interval is $O\left(\frac{\log(1/\epsilon')}{\log\log(1/\epsilon')}\right)$ and $O\left(m\left(\frac{\log(1/\epsilon')}{\log\log(1/\epsilon')}\right)^2\right)$, respectively. Furthermore, by the error accmulation in Lemma 14, we choose $\epsilon' = \epsilon/t\,(\|\mathcal{L}\|_{\mathrm{be}})$ in order to bound the overall error by ϵ.

In addition, since we need to invoke $e^{-iH_1\tau}$ once every step, the invoking number equals to M and is hence bounded as claimed. ◀

4.2 Comparison of the simulation complexity with and without interaction picture

In this subsection, we compare the complexity with simulations of Lindblad dynamics with and without the interaction picture. For the Lindbladian decomposition shown in Eq. (65), suppose we have access to the oracles U_{H_1},$U_{H_2(t)}$, and U_{L_j}. According to Theorem 11, a direct simulation involves a time complexity

$$C_{\mathrm{direct}} = O\left(t(C_1+C_2)(\alpha_{L_1}+\alpha_{L_2})(\frac{\log\left(t(\alpha_{L_1}+\alpha_{L_2})/\epsilon\right)}{\log\log\left(t(\alpha_{L_1}+\alpha_{L_2})/\epsilon\right)})^2\right) \tag{75}$$

where $\alpha_1 = \left\|\mathcal{L}_1(t)\right\|_{\mathrm{be},1}, \alpha_{L_2} = \left\|\mathcal{L}_2(t)\right\|_{\mathrm{be},1}$; C_1 and C_2 representing the gate complexity of implement U_{H_1} and the maximum gate complexity of implement $U_{H_2(t)}, U_{L_j}$ respectively.

Meanwhile for the simulation algorithm in interaction picture, the time complexity is given by the following theorem.

▶ **Theorem 16** (Gate complexity of Lindbladian simulation in the interaction picture)**.** *Suppose we are given U_{H_1},$U_{H_2(t)}$ and U_{L_j} block encoding of $H_1, H_2(t)$ and L_j respectively, such that e^{-iHs} is approximated to error ϵ using $C_{e^{-iH_1 s}}[\epsilon] \in \mathcal{O}\left(|s|\log^\gamma(s/\epsilon)\right)$ gates for some $\gamma > 0$ and any $|s| \geq 0$.*

For all $t > 0$, the time-evolution Eq. (70) *may be approximated to error ϵ with gate complexity*

$$\begin{aligned} &C_{\mathrm{interact}} \\ &= \mathcal{O}\left(\alpha_{L_2} t\left(C_2 + C_{e^{-iA/\alpha_{L_2}}}\left[\frac{\epsilon}{\alpha_{L_2} t\log\left(\alpha_{L_2}\right)}\right]\log\left(\frac{t\left(\alpha_{L_1}+\alpha_{L_2}\right)}{\epsilon}\right)\right)\frac{\log\left(\alpha_{L_2} t/\epsilon\right)}{\log\log\left(\alpha_{L_2} t/\epsilon\right)}\right) \\ &= \mathcal{O}\left(\alpha_{L_2} t\left(C_2 + C_{e^{-iA/\alpha_{L_2}}}[\epsilon]\right)\mathrm{polylog}\left(t\left(\alpha_{L_1}+\alpha_{L_2}\right)/\epsilon\right)\right) \end{aligned} \tag{76}$$

where $\alpha_1 = \left\|\mathcal{L}_1(t)\right\|_{\mathrm{be},\infty}, \alpha_{L_2} = \left\|\mathcal{L}_2(t)\right\|_{\mathrm{be},\infty} = \left\|\mathcal{L}_{2,I}(t)\right\|_{\mathrm{be},\infty}$.

The proof follows by using $\alpha_{L_1}, \alpha_{L_2,I}$ to substitute α_A and α_B in Theorem 7 in [41], respectively.

We highlight that the assumption $C_{e^{-iH_1 s}}[\epsilon] = O\left(|s|\log^\gamma(s/\epsilon)\right)$ imposes strong requirement on simulating the H_1 dynamics. With Hamiltonian simulation algorithm [5], gate complexity should be $C_{e^{-iH_1 s}}[\epsilon] = \tilde{O}(||H_1||s)$. But here the assumption removes the $||H_1||$ dependence. This implies that the simulation of H_1 is supposed to be easy, the dynamics can be fast-forwarded. Nevertheless this assumption is valid in some common settings [41], for instance when H_1 is diagonal. Another assumption is Eq. (64), which implies that $\alpha_2 \ll \alpha_1$. By comparing Eq. (75) and Eq. (76) with this relation, we find the simulation strategy using the interacting picture has a better gate complexity. As long as these two assumptions hold, the simulation algorithm in the interaction picture can serve as an alternative to reduce the simulation complexity.

5 The Optimization Algorithm for Quantum Optimal Control

In this section, we present our main results for finding first- and second-order stationary points of the optimization problem induced by the quantum optimal control problem (2), which in general is nonconvex. We consider the accelerated gradient descent (AGD) method [27]. A key departure from a direct implement of AGD is that the gradient has to be estimated using the quantum algorithm [21], in which case, the gradient input is subject to noise. We believe that this result may be of general interest to the optimization community.

▶ **Theorem 17.** *Assume that the function $f(\cdot)$ is ℓ-smooth and ϱ-Hessian Lipschitz. There exists an absolute constant $c_{\max}$ such that for any $\delta > 0, \epsilon \leq \frac{\ell^2}{\varrho}, \Delta_f \geq f(\mathbf{x}_0) - f^\star$, if $\chi = \max\left\{1, \log \frac{d\ell\Delta_f}{\varrho\epsilon\delta}\right\}$, $c \geq c_{\max}$ and such that if we run modified PAGD ([26, Algorithm 2]) with the choice of parameters in [26, Appendix C.1] using an approximate gradient $\hat{\nabla} f(x)$ with error bounded at every step: $\|\nabla f(x) - \hat{\nabla} f(x)\| \leq \epsilon_g$ with*

$$\epsilon_g = \frac{\varrho^{1/8}}{\sqrt{2}\ell^{1/4}\chi^{3/2}c^{3/2}}\epsilon^{9/8}, \tag{77}$$

then with probability at least $1-\delta$, one of the iterates $\mathbf{x}_t$ will be an ϵ-first order stationary point in the following number of iterations:

$$O\left(\frac{\ell^{1/2}\varrho^{1/4}\left(f\left(\mathbf{x}_0\right) - f^*\right)}{\epsilon^{7/4}}\log^6\left(\frac{d\ell\Delta_f}{\varrho\epsilon\delta}\right)\right). \tag{78}$$

Furthermore, if the error bound of the gradient is chosen as, $\epsilon_g = \frac{\delta\chi^{-11}c^{-16}}{64\ell}\frac{\epsilon^3}{\sqrt{d}}\frac{1}{\Delta_f}$, then with probability at least $1-\delta$, one of the iterates $\mathbf{x}_t$ will be an ϵ-second order stationary point.

The proof of this theorem can be found in the full version of this paper [26, Appendix C.7]. Note that the complexity $\tilde{O}(1/\epsilon^{7/4})$ in [27] is the currently best-known result for finding first- and second-order stationary points using only gradient queries, and there is not much space to improve as [11] proved a lower bound $\Omega(1/\epsilon^{12/7})$ for deterministic algorithms with gradient queries when the function is gradient- and Hessian-Lipschitz. Our error bound $\tilde{O}(1/\epsilon^{9/8})$ in (77) is optimal (up to poly-logarithmic factors) for PAGD because up to a concentration inequality, it can give an algorithm for stochastic gradient descent with complexity $\tilde{O}(1/\epsilon^{7/4} \cdot (1/\epsilon^{9/8})^2) = \tilde{O}(1/\epsilon^4)$, which is optimal as there is a matching lower bound $\Omega(1/\epsilon^4)$ [3]. In other words, if the error $\epsilon^{9/8}$ can be further improved, it implies an algorithm for finding stationary points with better convergence than [27], the current state-of-the-art work on this.

The AGD algorithm relies on an estimate of the gradient. Toward this end, we first show that the objective function (11) from the quantum control problem is essentially a polynomial. The polynomial nature of the objective function allows us to use high-order finite difference methods to compute the gradient. In particular, a centered difference scheme with $2m+1$ points will produce an exact gradient for a polynomial of degree $2m$.

▶ **Lemma 18.** *Assume that the control function is expressed as a linear combination of shape function $b_j(t)$: $u(t) = \sum_{j=0}^{N} u_j b_j(t)$ and let $\boldsymbol{u} = (u_0, u_1, \ldots, u_N)$. Then the expectation in Eq. (11) from the Lindblad simulation algorithms from the previous section is a polynomial with degree $d = O\left(T \operatorname{polylog}\frac{1}{\epsilon}\right)$.*

Proof. We begin by examining the time-dependent unitary $V(0,t)$ in Duhamel's representation. Specifically, from Eq. (28), we see that the Dyson series approximation yields a polynomial of degree at most K. In addition, in the Kraus form approximation in Eq. (31),

the operators $\mathcal{L}_{\mathrm{J}}(s)$ do not involve the control variable $\boldsymbol{u}$. Overall, the approximation $\mathcal{G}_K(t)$ in Eq. (31) constitutes a polynomial of degree at most K^2. Therefore, after applying $\mathcal{G}_K(\delta)$ for T/δ times to approximate the density operator at time T, we obtain a polynomial of degree at most $T\mathrm{polylog}\frac{1}{\epsilon}$. Here we have used the fact that $K = \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}$. Furthermore, when the gradient estimation algorithm in Lemma 8 is applied, the query complexity $\widetilde{O}\left(\frac{m}{\epsilon}\right)$ in Lemma 8 becomes $\widetilde{O}(T/\epsilon)$. ◀

6 Proof of Main Theorem

Finally, we outline the proof of our main theorem (Theorem 1). We first summarize our quantum algorithm as follows,

Algorithm 1 Quantum Algorithm for Open System Quantum Control.

1: Given $k_{\max}, \epsilon_g$ as in Theorem 17; set $u(t) = 0$
2: **for** t = 0,1,...,$k_{\max}$ **do**
3: Use Theorem 11 and strategy in Section 2.2.3 to construct the phase oracle for $\widetilde{J}_1(\boldsymbol{u})$;
4: Use Lemma 9 to estimate $\boldsymbol{g}^{(k)} \approx \nabla J\left(\boldsymbol{u}^{(k)}\right)$ with $||\boldsymbol{g}^{(k)} - J\left(\boldsymbol{u}^{(k)}\right)|| \leq \epsilon_g$;
5: Update control variable with one step of modified PAGD ([26, Algorithm 2]);
6: **end for**

Now, we restated the main theorem and give its proof:

▶ **Theorem 19** (main theorem, restated). *Assume there are n_{c} control functions $u_\beta(t) \in \mathrm{C}^2([0,T])$. Further assume*[4] *that $\|H_0\|, \|\mathcal{O}\|, \|\mu_\beta\|, \|L_j\| \leq 1$, and $\alpha \geq 2/T$. There exists a quantum algorithm that, with probability at least $2/3$*[5]*, solves problem (2) by:*

- *reaching a first-order stationary point $\|\nabla f\| < \epsilon$ with (1) using $\widetilde{O}\left(\frac{n_{\mathrm{c}}\|\mathcal{L}\|_{be,1}T}{\epsilon^{23/8}}\Delta_f\right)$ queries to $\mathcal{P}_{H_0}$ and $\mathcal{P}_{\mu_\beta}$, $\beta = 1, 2, \ldots, n_{\mathrm{c}}$, and $\widetilde{O}\left(mn\frac{n_{\mathrm{c}}\|\mathcal{L}\|_{be,1}T}{\epsilon^{23/8}}\Delta_f + n\frac{T^{3/2}}{\epsilon^{9/4}}\Delta_f\right)$ additional 1- and 2-qubit gates; or*
- *reaching a second-order stationary point using $\widetilde{O}\left(\frac{n_{\mathrm{c}}\|\mathcal{L}\|_{be,1}T^{7/4}}{\epsilon^{5}}\Delta_f\right)$ queries to $\mathcal{P}_{H_0}$ and $\mathcal{P}_{\mu_\beta}$, $\beta = 1, 2, \ldots, n_{\mathrm{c}}$ and $\widetilde{O}\left(mn\frac{n_{\mathrm{c}}\|\mathcal{L}\|_{be,1}T^{7/4}}{\epsilon^{5}}\Delta_f + n\frac{T^{3/2}}{\epsilon^{9/4}}\Delta_f\right)$ additional 1- and 2-qubit gates.*

Here n_{c} and m are respectively the number of control variables and jump operators.

Proof. We denote gate complexity of control $U_{\mathcal{O}}$ by $C_{\mathrm{c}-U_{\mathcal{O}}}$, gate complexity of U_H, U_{L_j} by $C_{U_H,U_{L_j}}$, and gate complexity of quantum simulation by $C_{\varrho(t)}$. The gate complexity of preparing a state after Lindblad evolution is given by Theorem 11,

$$C_{\varrho(t)} = O\left(\|\mathcal{L}\|_{\mathrm{be},1}\frac{\log\left(\|\mathcal{L}\|_{\mathrm{be},1}/\epsilon\right)}{\log\log\left(\|\mathcal{L}\|_{\mathrm{be},1}/\epsilon\right)}\right)C_{U_H,U_{L_j}} + \tilde{O}\left(m\|\mathcal{L}\|_{\mathrm{be},1}n\right). \tag{79}$$

With copies of states $\varrho(t)$ and access to control $U_{\mathcal{O}}$ oracle, we can construct the gradient following Section 2.2.3. According to that section, we can construct the probability oracle with $\varrho(t)$, construct the phase oracle with probability oracle, and calculate the gradient with the phase oracle. The corresponding complexity is listed below:

[4] More generally, if $\|H_0\|, \|\mu\| = \Theta(\Lambda)$, it is equivalent to enlarge the time duration T by a factor $O(\Lambda)$.
[5] Using standard techniques, the success probability can be boosted to a constant arbitrarily close to 1 while only introducing a logarithmic factor in the complexity.

$$C_{U_{J_1}} = C_{\varrho(t)} + O(1) + C_{c-U_O}, \tag{80}$$

$$C_{\mathcal{O}_{J_1}} = O(\log 1/\epsilon) C_{U_{J_1}}, \tag{81}$$

$$C_{\nabla J} = \tilde{O}(n_{\mathrm{c}} T \log(N/\gamma)/\epsilon) C_{\mathcal{O}_{J_1}} + \tilde{O}(N), \tag{82}$$

where $1-\gamma$ is the successful probability of obtaining a gradient, n_{c} is the number of parameters, and N is the time steps $N = O\left(t^{3/2}/\epsilon^{1/2}\right)$ as in [35, Corollary 2.2]. Here we define $\gamma = \nu/k$, where ν is a small finite number and k is the iteration steps, which we will give below. Combining them together, we have

$$\begin{aligned} C_{\nabla J} = \tilde{O}\left(n_{\mathrm{c}} \frac{\|\mathcal{L}\|_{\mathrm{be},1} T \log \frac{N}{\gamma}}{\epsilon}\right) C_{U_H, U_{L_j}} + \tilde{O}(n_{\mathrm{c}} \frac{T \log \frac{N}{\gamma}}{\epsilon}) C_{\mathrm{c}-U_O} \\ + \tilde{O}(mnn_{\mathrm{c}} \frac{\|\mathcal{L}\|_{\mathrm{be},1} T \log \frac{N}{\gamma}}{\epsilon} + N). \end{aligned} \tag{83}$$

Here we reassign the gradient noise ϵ with ϵ_g to distinguish from the other errors.

$$\begin{aligned} C_{\nabla J} = \tilde{O}\left(n_{\mathrm{c}} \frac{\|\mathcal{L}\|_{\mathrm{be},1} T \log \frac{N}{\gamma}}{\epsilon_g}\right) C_{U_H, U_{L_j}} + \tilde{O}(n_{\mathrm{c}} \frac{T \log \frac{N}{\gamma}}{\epsilon_g}) C_{\mathrm{c}-U_O} \\ + \tilde{O}(mnn_{\mathrm{c}} \frac{\|\mathcal{L}\|_{\mathrm{be},1} T \log \frac{N}{\gamma}}{\epsilon_g} + N). \end{aligned} \tag{84}$$

With modified PAGD method ([26, Algorithm 2]), we can find a first or second order ϵ-stationary point within

$$k = \tilde{O}\left(\frac{\ell^{1/2} \varrho^{1/4} \left(f\left(\mathbf{x}_0\right) - f^*\right)}{\epsilon^{7/4}}\right) \tag{85}$$

iterations by Theorem 17. For first ϵ-order stationary point, the gradient noise tolerance is $\epsilon_g = \frac{\varrho^{1/8}}{\sqrt{2}\ell^{1/4}\chi^{3/2}c^{3/2}}\epsilon^{9/8}$. For second order ϵ-order stationary point, it is $\epsilon_g = \frac{\delta\chi^{-11}c^{-16}}{64\ell}\frac{\epsilon^3}{\sqrt{d}}\frac{1}{\Delta_f}$.

In each iteration, we need to calculate ∇J once and calculate J once. Noticing that $C_J = O(C(\varrho(t)))$, we have

$$C_{\mathrm{total}} = k \times (C_{\nabla J} + C_{\varrho(t)}). \tag{86}$$

Substitute Eqs. (79) and (84), (85) into Eq. (86) we finish the proof. Notice that in optimization, dimension $d = N$, and here we regard ℓ and ϱ as constants. ◀

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