Quantum Algorithm for Time-Dependent Hamiltonian Simulation by Permutation Expansion

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We present a quantum algorithm for the dynamical simulation of time-dependent Hamiltonians. Our method involves expanding the interaction-picture Hamiltonian as a sum of generalized permutations, which leads to an integral-free Dyson series of the time-evolution operator. Under this representation, we perform a quantum simulation for the time-evolution operator by means of the linear combination of unitaries technique. We optimize the time steps of the evolution based on the Hamiltonian's dynamical characteristics, leading to a gate count that scales with an L^1 -norm-like scaling with respect only to the norm of the interaction Hamiltonian, rather than that of the total Hamiltonian. We demonstrate that the cost of the algorithm is independent of the Hamiltonian's frequencies, implying its advantage for systems with highly oscillating components, and for time-decaying systems the cost does not scale with the total evolution time asymptotically. In addition, our algorithm retains the near optimal $\log(1/\epsilon)/\log \log(1/\epsilon)$ scaling with simulation error ϵ .

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I. INTRODUCTION

The problem of simulating quantum systems, whether it is to study their dynamics, or to infer their salient equilibrium properties, was the original motivation for quantum computers [1] and remains one of their major potential applications [2,3]. Classical algorithms for this problem are known to be grossly inefficient. Nonetheless, a significant fraction of the world's computing power today is spent on solving instances of this problem—a reflection on their importance [4–6].

An important class of quantum simulations that is known to be particularly challenging, and is the focus of this work, is that of time-dependent quantum processes, which are at the heart of many important quantum phenomena. These include, for example, quantum control schemes [7], transition states of chemical reactions [8], analog quantum computers such as quantum annealers [9], and the quantum approximate optimization algorithm [10]. Devising state-of-the-art resource efficient quantum algorithms

to simulate these types of processes on quantum circuits is therefore a very worthy cause: it will allow for the studying of said phenomena in a controllable and vastly more illuminating manner.

In the literature, a number of quantum algorithms designed to simulate the dynamics of time-dependent quantum many-body Hamiltonians already exist. However, most of them are variants of algorithms that suit time-independent Hamiltonians but lack optimizations for dynamical ones. For example, Hamiltonians based on the Lie-Trotter-Suzuki decomposition were developed in Refs. [11,12], where the complexity scales polynomially with error. More recent advances [13,14] improve it to a logarithmic error scaling, which directly lead to applications in time-dependent Hamiltonian simulations [15,16]. A recent study by Berry *et al.* [17] improves the Hamiltonian scaling to L^1 -norm, by considering the dynamical properties of the time-dependent Hamiltonian. However, these mostly comprise of slicing the dynamics into a sequence of “quasi-static” steps, each of which implementing a static quantum simulation module. In addition, all the abovementioned algorithms assume a time-dependent oracle—a straightforward but not necessarily practical assumption that can obscure the true complexity of the simulation when physical models are considered.

The suboptimality that characterizes existing quantum algorithms can be attributed mainly to the fact that the

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time-evolution operator for time-dependent Hamiltonians is a more intricate entity than its time-independent counterpart (this matter is discussed in more detail below). While in the time-independent case the Schrödinger equation can be formally integrated, the time-evolution unitary operator for time-dependent systems is given in terms of a Dyson series [18]—a perturbative expansion, wherein each summand is a multidimensional integral over a time-ordered product of the (usually interaction-picture) Hamiltonian at different points in time. These time-ordered integrals pose multiple algorithmic and implementation challenges.

In this paper, we provide a quantum algorithm for simulating a time-dependent Hamiltonian dynamics. This algorithm invokes a separation of the Hamiltonian $H(t)$ into a sum of a static diagonal part H_0 and a dynamical part $V(t)$, i.e., $H(t) = H_0 + V(t)$, and switches to the interaction picture with respect to H_0 . The target evolution operator becomes a product of an interaction-picture unitary $U_I(t)$ followed by a diagonal unitary $e^{-iH_0 t}$ that can be simulated efficiently. The interaction Hamiltonian $V(t)$ is expanded as a sum of generalized permutations, and the resulting Dyson series of the evolution operator $U_I(t)$ becomes an integral-free representation [19] with the notion of divided differences, which is a well-studied quantity [20–25]. The divided differences have an intuition of discretized derivatives and is closely related to polynomial interpolations [20]. We refer the reader to Appendix A for a short summary of the notion of the divided differences. Under this representation, we use the linear combination of unitaries (LCU) method [14] to simulate $U_I(t)$ with a truncated Dyson series. We find a partitioning scheme that determines the duration of the time steps along the simulation. Following this procedure, in general, each time interval has a different duration that is determined from the Hamiltonian's dynamical characteristics and can lead to a substantially fewer number of steps as compared to using identical-length simulation segments, typically used in quantum simulation algorithms. We analyze the implementation gate and qubit costs and discuss the circumstances under which our simulation algorithm provides improvements over the state of the art. Specifically, our algorithm is independent of the oscillation frequencies of the Hamiltonian. This is in stark contrast to existing algorithms that have dependence on $||dH(t)/dt||$, which grows with oscillation rates. Another class of Hamiltonians for which our algorithm is preferred over others is those with exponential decays in time. We show that, for these systems, our algorithms require asymptotically a finite number of steps that does not scale with the evolution time, leading in turn to an exponential saving comparing to the linear scaling in existing approaches. Moreover, the cost with Hamiltonian norm only mainly depends on the interaction Hamiltonian $V(t)$ and not the total Hamiltonian $H(t)$ [17]. This also indicates an advantage of the algorithm when the time-dependent Hamiltonian is dominant by a static part.

The paper is organized as follows. In Sec. II, we review the permutation expansion method that leads to an integral-free representation for the Dyson series, as introduced in Ref. [19]. In Sec. III, we present in detail the simulation algorithm that combines the integral-free expression of the evolution operator with the LCU method, and analyze the circuit costs. We highlight the main advantages of our algorithm in Sec. III D 3. In Sec. III E, we address the cases when the exponential-sum expansion of the time dependence is not exact and estimate the error that stems from a finite sum approximation. Finally, we give a brief summary for our methods and results in Sec. V.

II. PERMUTATION EXPANSION METHOD FOR TIME-DEPENDENT HAMILTONIANS

In this section, we briefly describe the integral-free Dyson series expression of the evolution operator, derived from a permutation expansion of the time-dependent Hamiltonian [19]. Without loss of generality [26], we expand a general time-dependent Hamiltonian in terms of products of time-dependent diagonal matrices, $D_i(t)$, and permutation operators, P_i , i.e.,

$$H(t) = \sum_{i=0}^M D_i(t) P_i, \quad (1)$$

where $P_0 \equiv 1$. This decomposition can be done efficiently as long as M scales polynomially with $\log d$, where d is the dimension of the Hamiltonian. We decompose each diagonal matrix into a finite sum of exponential functions, i.e.,

$$D_i(t) = \sum_{k=1}^{K_i} \exp(\Lambda_i^{(k)} t) D_i^{(k)}, \quad (2)$$

where $\Lambda_i^{(k)}$ and $D_i^{(k)}$ are complex diagonal matrices with diagonal elements being

$$\lambda_{i,z}^{(k)} \equiv \langle z | \Lambda_i^{(k)} | z \rangle, \quad (3)$$

$$d_{i,z}^{(k)} \equiv \langle z | D_i^{(k)} | z \rangle, \quad (4)$$

in some basis $\{|z\rangle\}$ (the basis in which D_0 is diagonal) and K_i indicates the number of terms in the exponential decomposition for $D_i(t)$. This can be done for many cases when the time dependencies are simple combinations of exponential terms. For simplicity, we assume here that the K_i are finite, and address the most general time dependence in detail in Sec. III E and refer to various algorithms [27–31] for efficiently finding an exponential sum approximation of a function.

For a lighter notation, we set $K_i = K$ for all i . We can evaluate the time-evolution operator $U(t)$ corresponding to $H(t)$ as

$$\begin{aligned} U(t) &\equiv \mathcal{T} \exp \left[-i \int_0^t H(t') dt' \right] \\ &= \sum_{q=0}^{\infty} (-i)^q \int_0^t d\tau_q \cdots \int_0^{\tau_2} d\tau_1 H(\tau_q) \cdots H(\tau_1) \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^t d\tau_q \cdots \\ &\quad \times \int_0^{\tau_2} d\tau_1 \exp(\Lambda_{i_q}^{(k_q)} \tau_q) D_{i_q}^{(k_q)} P_{i_q} \cdots \\ &\quad \times \exp(\Lambda_{i_1}^{(k_1)} \tau_1) D_{i_1}^{(k_1)} P_{i_1}, \quad (5) \end{aligned}$$

where $\mathbf{i}_q = \{i_q, \dots, i_1\}$ and $\mathbf{k}_q = \{k_q, \dots, k_1\}$ are multi-indices. The action of $U(t)$ on a basis vector $|z\rangle$ is

$$\begin{aligned} U(t)|z\rangle &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^t d\tau_q \cdots \int_0^{\tau_2} d\tau_1 \\ &\quad \times \exp(\lambda_{i_q, z_{i_q}}^{(k_q)} \tau_q + \cdots \lambda_{i_1, z_{i_1}}^{(k_1)} \tau_1) d_{i_q, z_{i_q}}^{(k_q)} \cdots d_{i_1, z_{i_1}}^{(k_1)} \\ &\quad \times P_{i_q} \cdots P_{i_1} |z\rangle \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^t d\tau_q \cdots \int_0^{\tau_2} d\tau_1 \\ &\quad \times \exp(\lambda_{i_q, z_{i_q}}^{(k_q)} \tau_q + \cdots \lambda_{i_1, z_{i_1}}^{(k_1)} \tau_1) d_{i_q, z}^{(k_q)} P_{i_q} |z\rangle, \quad (6) \end{aligned}$$

where $|z_{i_j}\rangle \equiv P_{i_j} \cdots P_{i_1} |z\rangle$ with j ranging from 1 to q , and $\lambda_{i_j, z_{i_j}}^{(k_j)} (d_{i_j, z_{i_j}}^{(k_j)})$ is the z_{i_j} th diagonal element of $\Lambda_{i_j}^{(k_j)} (D_{i_j}^{(k_j)})$. We use P_{i_q} as shorthand for $P_{i_q} \cdots P_{i_1}$, and similarly $d_{i_q, z}^{(k_q)} \equiv d_{i_q, z_{i_q}}^{(k_q)} \cdots d_{i_1, z_{i_1}}^{(k_1)}$. Figure 1 illustrates the accumulative actions of $D_i^{(k)} P_i$ on a basis vector $|z\rangle$.

To proceed, we use the following identity to simplify the expression in terms of divided differences. It is a variant of Hermite-Genocchi formula [20] applying to the exponential function.

Identity 1. For $\lambda_1, \dots, \lambda_q \in \mathbb{C}$,

$$\int_0^1 ds_q \cdots \int_0^{s_2} ds_1 e^{(\lambda_1 s_1 + \cdots + \lambda_q s_q)} = e^{[x_1, \dots, x_q, 0]}, \quad (7)$$

where $x_j = \sum_{l=j}^q \lambda_l$ and $e^{[x_1, \dots, x_q, 0]}$ is the divided difference of the exponential function with inputs $x_1, \dots, x_q, 0$. (The case with $q = 1$ can be shown by explicit integration, and the identity follows by induction. For more details, see Ref. [19].)

With this property, the multidimensional integration in the time-evolution operator can be simplified as

$$\begin{aligned} U(t)|z\rangle &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^t d\tau_q \cdots \int_0^{\tau_2} d\tau_1 \\ &\quad \times \exp(\lambda_{i_q, z_{i_q}}^{(k_q)} \tau_q + \cdots \lambda_{i_1, z_{i_1}}^{(k_1)} \tau_1) d_{i_q, z}^{(k_q)} P_{i_q} |z\rangle \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^1 ds_q \cdots \int_0^{s_2} ds_1 \\ &\quad \times \exp[t(\lambda_{i_q, z_{i_q}}^{(k_q)} s_q + \cdots \lambda_{i_1, z_{i_1}}^{(k_1)} s_1)] d_{i_q, z}^{(k_q)} P_{i_q} |z\rangle \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{[x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(k_q)} P_{i_q} |z\rangle, \quad (8) \end{aligned}$$

where $x_j = \sum_{l=j}^q \lambda_{i_l, z_{i_l}}^{(k_l)}$. The second equality uses the change of variable $d\tau = t ds$, and the last equality follows from Identity 1 and the identity of $t^q e^{[x_0, \dots, x_q]} = e^{[x_0, \dots, x_q, 1]}$. By completing the basis, we get

$$\begin{aligned} U(t) &= \sum_z U(t)|z\rangle \langle z| \\ &= \sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{[x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(k_q)} P_{i_q} |z\rangle \langle z|. \quad (9) \end{aligned}$$

This is an integral-free expression for the unitary time-evolution operator of the time-dependent Hamiltonian $H(t)$. We will later approximate the unitary by truncating the series at some order $q = Q$ that scales as $\mathcal{O}[\log(1/\epsilon)/\log\log(1/\epsilon)]$ [14], where ϵ is the required accuracy.

III. TIME-DEPENDENT HAMILTONIAN SIMULATION ALGORITHM

A time-dependent Hamiltonian $H(t)$ can be expressed as a sum of two Hamiltonians—a time-independent H_0 and a dynamical $V(t)$, i.e.,

$$H(t) = H_0 + V(t). \quad (10)$$

In many practical models, H_0 represents a static and simple Hamiltonian that is often diagonal in a known basis (which we will identify with the computational basis). Hence, hereafter, we assume that H_0 is a diagonal operator with real diagonal elements. The $V(t)$ component represents the nontrivial interactions between subsystems. Assume [32] that H_0 is diagonal in the computational basis $\{|z\rangle\}$. We

FIG. 1. The actions of a sequence of generalized permutations. This figure gives a pictorial illustration on how the elements of the diagonal matrices are picked up when interleaving with permutations. In this example, we have $q = 2$.

switch to the interaction picture, i.e.,

$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle \rightarrow \frac{d}{dt}|\psi_I(t)\rangle = -iH_I(t)|\psi_I(t)\rangle, \quad (11)$$

where

$$|\psi_I(t)\rangle = e^{iH_0 t}|\psi(t)\rangle \quad \text{and} \quad H_I(t) = e^{iH_0 t}V(t)e^{-iH_0 t}. \quad (12)$$

The Schrödinger-picture unitary operator $U(t)$, satisfying $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, is equivalent to a time-ordered matrix exponential followed by a diagonal unitary, i.e.,

$$\begin{aligned} U(t) &= e^{-iH_0 t} \mathcal{T} \exp \left[-i \int_0^t H_I(t') dt' \right] \\ &= e^{-iH_0 t} \mathcal{T} \exp \left[-i \int_0^t e^{iH_0 t'} V(t') e^{-iH_0 t'} dt' \right]. \end{aligned} \quad (13)$$

Hence, the simulation of $U(t) = e^{-iH_0 t} U_I(t)$ consists of two parts—a complicated $U_I(t)$ and a simple diagonal unitary $e^{-iH_0 t}$. The simulation of $e^{-iH_0 t}$ can be achieved with a gate cost that scales only linearly with the locality of H_0 (the highest weight of terms in H_0). When we write $H_0 = \sum_{\gamma=0}^L J_{\gamma} Z_{\gamma}$, where each Z_{γ} is some tensor product of (single-qubit) Pauli-Z operators acting on at most d qubits (locality d), it can be shown that the gate cost scales as $\mathcal{O}(Ld)$ [33,34]. Therefore, the main focus of our simulation is on U_I .

We next provide an overview of the simulation algorithm in Sec. III A. In Sec. III B, we incorporate the LCU framework with the permutation expansion method. Section III C 2 provides the state preparation operation and Sec. III D evaluates the simulation cost for the whole procedure.

A. An overview of the algorithm

Our proposed simulation algorithm consists of a permutation expansion procedure for U_I and the LCU method for the quantum simulation. In Sec. III B, we explain in detail the essential ingredients for merging these two approaches. Before delving into technical details, we provide an overview of the algorithm in this section.

Given a time-dependent Hamiltonian $H(t)$, we first decompose $H(t)$ into a sum of a static diagonal term H_0 (if it exists) and a dynamical term $V(t)$. We switch to an interaction picture so that the target unitary evolution $U(T)$ over a period T becomes

$$\begin{aligned} U(T) &= e^{-iH_0 T} \mathcal{T} \exp \left[-i \int_0^T e^{iH_0 t} V(t) e^{-iH_0 t} dt \right] \\ &\equiv e^{-iH_0 T} U_I(T). \end{aligned} \quad (14)$$

Therefore, the simulation of $U(T)$ is equivalent to applying $U_I(T)$ followed by $e^{-iH_0 T}$. Since the diagonal unitary $e^{-iH_0 T}$ can be efficiently simulated, we focus on $U_I(T)$ hereafter.

Let us expand $V(t)$ as a sum of permutations as

$$V(t) = \sum_{i=0}^M D_i(t) P_i, \quad (15)$$

where the P_i are permutations ($P_0 \equiv \mathbb{1}$) and the $D_i(t)$ are some diagonal matrices that are expressed as exponential sums, i.e.,

$$D_i(t) = \sum_{k=1}^K \exp(\Lambda_i^{(k)} t) D_i^{(k)}. \quad (16)$$

Here $\Lambda_i^{(k)}$ and $D_i^{(k)}$ are some complex diagonal matrices. Partition $U_I(T)$ into r segments $U_I(T, t_{r-1}) \cdots U_I(t_1, 0)$,

whose respective durations Δt_w , $w = 0, \dots, r-1$, are determined by the partitioning scheme given in Sec. III B and the time markers t_w are defined as $t_w = \sum_{l=0}^{w-1} \Delta t_l$. The total number of steps is denoted as r . The evolution operator from t_w to $t_w + \Delta t_w$ is expressed as

$$U_I(t_w + \Delta t_w, t_w) = \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sum_{x=\pm} (-i)^q \times \frac{[(e^{\Delta t_w \lambda} - 1)/\lambda]^q}{2q!} \Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w) P_{\mathbf{i}_q} \Phi_{\mathbf{i}_q, x}^{(\mathbf{k}_q, w)} \quad (17)$$

with

$$\Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w) = \|D_{\mathbf{i}_q}^{(\mathbf{k}_q)}\|_{\max} e^{t_w \lambda_{(\mathbf{i}_q, \mathbf{k}_q)}} \dots \|D_{\mathbf{i}_1}^{(\mathbf{k}_1)}\|_{\max} e^{t_w \lambda_{(\mathbf{i}_1, \mathbf{k}_1)}}, \quad (18)$$

where $\|\cdot\|_{\max}$ is the max norm, $\lambda_{(i,k)} = \max_z \text{Re}(\langle z | \Lambda_i^{(k)} | z \rangle)$ is the maximum real part of $\Lambda_i^{(k)}$, and $\lambda = \max_{i,k} \{\lambda_{(i,k)}\}$. Here, $\Phi_{\mathbf{i}_q, \pm}^{(\mathbf{k}_q, w)}$ are some diagonal unitaries as derived later in Eq. (38) and each $P_{\mathbf{i}_q}$ is a unique product of permutations. Note that the above evolution operators are given as a LCU. We provide a review for the LCU method in Appendix C. We set the truncation order Q to be

$$Q = \mathcal{O}\left(\frac{\log(r/\epsilon)}{\log \log(r/\epsilon)}\right), \quad (19)$$

where ϵ is the overall simulation accuracy.

To implement the LCU routine for each $U_I(t_w + \Delta t_w, t_w)$, we require preparing a state

$$|\psi_0\rangle = \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sum_{x=0,1} \times \sqrt{\frac{[(e^{\Delta t_w \lambda} - 1)/\lambda]^q \Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w)}{2q!}} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle, \quad (20)$$

where $|\mathbf{i}_q\rangle$ represents Q quantum registers that each has dimension M and $|\mathbf{k}_q\rangle$ represents Q quantum registers that each has dimension K , and s is the normalization factor. Following the same notation as used in Appendix C, let us denote the state preparation unitary as B , i.e., $B|0\rangle^{\otimes 2Q+1} = |\psi_0\rangle$ (B is explicitly given in Sec. III C 2). Let us denote by V_c the control unitary such that

$$V_c |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle |\psi\rangle = |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle (-i)^q P_{\mathbf{i}_q} \Phi_{\mathbf{i}_q, x}^{(\mathbf{k}_q, w)} |\psi\rangle. \quad (21)$$

The oblivious amplitude amplification (OAA) involves interleaving the operator $W = (B^\dagger \otimes I) V_c (B \otimes I)$ as

$$A = -WRW^\dagger RW, \quad (22)$$

where $R \equiv I - 2(|0\rangle\langle 0| \otimes I)$. For each piece of the unitary, we implement A on the extended system $|0\rangle^{\otimes (2Q+1)} |\psi\rangle$. By construction, we have

$$\begin{aligned} & \| |A|0\rangle^{\otimes (2Q+1)} |\psi\rangle - |0\rangle^{\otimes (2Q+1)} U_I(t_w + \Delta t_w, t_w) |\psi\rangle \| \\ &= \mathcal{O}\left(\frac{\epsilon}{r}\right). \end{aligned} \quad (23)$$

This means that applying A effectively performs the unitary $U_I(t_w + \Delta t_w, t_w)$ on the main system $|\psi\rangle$, with error $\mathcal{O}(\epsilon/r)$. Combining r pieces of the procedure, it effectively simulates $U_I(T)$ with overall error $\mathcal{O}(\epsilon)$, i.e.,

$$\begin{aligned} & \| |A_{r-1} \dots A_1 A_0 |0\rangle^{\otimes (2Q+1)} |\psi\rangle - |0\rangle^{\otimes (2Q+1)} U_I(T) |\psi\rangle \| \\ &= \mathcal{O}(\epsilon), \end{aligned} \quad (24)$$

where A_w are the OAA operators for the corresponding piece of evolution. This implies that applying the sequence of A 's followed by the circuit for $e^{-iH_0 T}$ can approach the action of $U(T)$ to an arbitrary accuracy.

B. Permutation expansion for $U_I(t)$

In this section, we give a thorough introduction of the permutation expansion in the Dyson series and the conditions that arise from implementing the LCU method. We focus on addressing the interaction-picture unitary $U_I(t)$, i.e., the time-ordered operator in Eq. (13). Using the expansions introduced in Eqs. (15) and (16), we get

$$\begin{aligned} U_I(t) &\equiv \mathcal{T} \exp \left[-i \int_0^t e^{iH_0 t'} V(t') e^{-iH_0 t'} dt' \right] \\ &= \sum_{q=0}^{\infty} (-i)^q \int_0^t d\tau_q \dots \int_0^{\tau_2} d\tau_1 e^{iH_0 \tau_q} V(\tau_q) e^{-iH_0 \tau_q} \dots \\ &\quad \times e^{iH_0 \tau_1} V(\tau_1) e^{-iH_0 \tau_1}. \end{aligned} \quad (25)$$

We denote the basis in which H_0 is diagonal by $\{|z\rangle\}$ and its diagonal elements by $E_z = \langle z | H_0 | z \rangle$. The action of $U_I(t)$ on a basis vector $|z\rangle$ becomes

$$\begin{aligned} U_I(t) |z\rangle &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_0^t d\tau_q \dots \\ &\quad \times \int_0^{\tau_2} d\tau_1 \exp[(iE_{z_{\mathbf{i}_q}} - iE_{z_{\mathbf{i}_{q-1}}} + \lambda_{\mathbf{i}_q, z_{\mathbf{i}_q}}^{(k_q)}) \tau_q + \dots \\ &\quad + (iE_{z_{\mathbf{i}_1}} - iE_z + \lambda_{\mathbf{i}_1, z_{\mathbf{i}_1}}^{(k_1)}) \tau_1] d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle, \end{aligned} \quad (26)$$

where $E_{z_{\mathbf{i}_j}}$ is the $z_{\mathbf{i}_j}$ th diagonal element of H_0 , i.e., $E_{z_{\mathbf{i}_j}} = \langle z_{\mathbf{i}_j} | H_0 | z_{\mathbf{i}_j} \rangle$, and $|z_{\mathbf{i}_j}\rangle = P_{\mathbf{i}_j} |z\rangle$ with $P_{\mathbf{i}_j} = P_{i_j} \dots P_{i_1}$. By

Identity 1, this can be further simplified as

$$U_I(t)|z\rangle = \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{i[x_1, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle, \quad (27)$$

where

$$x_j = i(E_{z_{i_q}} - E_{z_{i_{j-1}}}) + \sum_{l=j}^q \lambda_{i_l, z_{i_l}}^{(k_l)}. \quad (28)$$

C. The LCU routine

To implement the LCU method for a quantum simulation of $U_I(T)$, we first decompose the overall simulation duration T into r pieces in sequence, i.e.,

$$\begin{aligned} U_I(T) &= U_I(T, t_{r-1}) U_I(t_{r-1}, t_{r-2}) \cdots U_I(t_1, 0) \\ &= \prod_{w=0}^{r-1} U_I(t_w + \Delta t_w, t_w), \end{aligned} \quad (29)$$

where the operators in the product of the last equation are understood to be ordered, $t_{w+1} = t_w + \Delta t_w$ and $t_0 \equiv 0$ and $t_r \equiv T$. The number of steps, r , and the step size, Δt_w , are to be determined. When acting on a computational basis state, each piece in the decomposition can be written as

$$\begin{aligned} U_I(t_w + \Delta t_w, t_w)|z\rangle &= \mathcal{T} \exp \left[-i \int_{t_w}^{t_w + \Delta t_w} H_I(t') dt' \right] |z\rangle \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \int_{t_w}^{t_w + \Delta t_w} d\tau_q \cdots \\ &\quad \times \int_{t_w}^{\tau_2} d\tau_1 \exp \left[\sum_{l=1}^q (iE_{z_{i_l}} - iE_{z_{i_{l-1}}} + \lambda_{i_l, z_{i_l}}^{(k_l)}) \tau_l \right] \\ &\quad \times d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle, \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \exp \left[t_w \sum_{l=1}^q (iE_{z_{i_l}} - iE_{z_{i_{l-1}}} + \lambda_{i_l, z_{i_l}}^{(k_l)}) \right] \\ &\quad \times \int_0^{\Delta t_w} d\tau'_q \cdots \\ &\quad \times \int_0^{\tau'_2} d\tau'_1 \exp \left[\sum_{l=1}^q (iE_{z_{i_l}} - iE_{z_{i_{l-1}}} + \lambda_{i_l, z_{i_l}}^{(k_l)}) \tau'_l \right] \\ &\quad \times d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \end{aligned}$$

$$\begin{aligned} &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \exp \left[t_w \sum_{l=1}^q (iE_{z_{i_l}} - iE_{z_{i_{l-1}}} + \lambda_{i_l, z_{i_l}}^{(k_l)}) \right] \\ &\quad \times e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \\ &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{-it_w (E_{z_{i_0}} - E_{z_{i_q}})} e^{t_w \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)}} \\ &\quad \times e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle, \end{aligned} \quad (30)$$

which has the same form as Eq. (27) except that the integration intervals are shifted (with $E_{z_{i_0}} \equiv E_z$). We can set

$$d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}(t_w) = d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} e^{t_w \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)}},$$

which leads to

$$\begin{aligned} U_I(t_w + \Delta t_w, t_w)|z\rangle &= \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{-it_w (E_{z_{i_0}} - E_{z_{i_q}})} \\ &\quad \times e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}(t_w) P_{\mathbf{i}_q} |z\rangle. \end{aligned} \quad (31)$$

To formulate the above expression in terms of a linear combination of unitaries, we need to evaluate the norms of $e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]}$ and $d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}(t_w)$. The norm of $d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}(t_w)$ is bounded by

$$\begin{aligned} |d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}(t_w)| &\leq \|D_{i_q}^{(k_q)}\|_{\max} e^{t_w \lambda_{i_q, k_q}} \cdots \|D_{i_1}^{(k_1)}\|_{\max} e^{t_w \lambda_{i_1, k_1}} \\ &= \Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w). \end{aligned} \quad (32)$$

The norm of the $e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]}$ can be bounded by using the following identity.

Identity 2. For any $q+1$ complex values $x_0, \dots, x_q \in \mathbb{C}$,

$$|e^{[x_0, \dots, x_q]}| \leq e^{[\text{Re}(x_0), \dots, \text{Re}(x_q)]} = \frac{e^{\xi}}{q!}, \quad (33)$$

where $\text{Re}(\cdot)$ denotes the real part of an input and $\xi \in [\min\{\text{Re}(x_0), \dots, \text{Re}(x_q)\}, \max\{\text{Re}(x_0), \dots, \text{Re}(x_q)\}]$.

The proof can be found in Appendix A. From Identity 2, we show in Appendix B that

$$\begin{aligned} |e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]}| &\leq e^{\Delta t_w [q\lambda, (q-1)\lambda, \dots, \lambda, 0]} \\ &= \frac{1}{q!} \left(\frac{e^{\Delta t_w \lambda} - 1}{\lambda} \right)^q \\ &\equiv \frac{\widetilde{\Delta t_w^q}}{q!}, \end{aligned} \quad (34)$$

where we have defined the quantity

$$\widetilde{\Delta t_w} \equiv \frac{e^{\Delta t_w \lambda} - 1}{\lambda}. \quad (35)$$

With these bounds, the factors in the expansion form in Eq. (31) can be written as

$$\begin{aligned} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(\mathbf{k}_q)}(t_w) \\ = \frac{\widetilde{\Delta t_w}^q}{q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w) \cos[\phi_{i_q, z}^{(\mathbf{k}_q)}] e^{i\theta_{i_q, z}^{(\mathbf{k}_q)}} \\ = \frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w) (e^{i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}} + e^{-i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}}), \end{aligned} \quad (36)$$

where

$$\phi_{i_q, z}^{(\mathbf{k}_q)} = \cos^{-1} \left[\frac{e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(\mathbf{k}_q)}(t_w)}{(\widetilde{\Delta t_w}^q / q!) \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w)} \right]$$

and

$$\theta_{i_q, z}^{(\mathbf{k}_q)} = \arg \left[\frac{e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(\mathbf{k}_q)}(t_w)}{(\widetilde{\Delta t_w}^q / q!) \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w)} \right].$$

The evolution operator from t_w to $t_w + \Delta t_w$ becomes

$$\begin{aligned} U_I(t_w + \Delta t_w, t_w) &= \sum_z U_I(t_w + \Delta t_w, t_w) |z\rangle \langle z| \\ &= \sum_z \sum_{q=0}^{\infty} \sum_{i_q} \sum_{\mathbf{k}_q} (-i)^q \frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w) \\ &\quad \times (e^{i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}} + e^{-i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}}) P_{i_q} |z\rangle \langle z| \\ &= \sum_{q=0}^{\infty} \sum_{i_q} \sum_{\mathbf{k}_q} \sum_{x=\pm} (-i)^q \frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w) P_{i_q} \Phi_{i_q, x}^{(\mathbf{k}_q, w)}, \end{aligned} \quad (38)$$

where $\Phi_{i_q, \pm}^{(\mathbf{k}_q, w)}$ are diagonal unitaries with diagonal elements being $e^{i(\pm\phi_{i_q, z}^{(\mathbf{k}_q)} + \theta_{i_q, z}^{(\mathbf{k}_q)})}$.

To implement the LCU method for simulating $U_I(t_w + \Delta t_w, t_w)$, we require a preparation of the state

$$\begin{aligned} |\psi_0\rangle &= \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sum_{i_q} \sum_{\mathbf{k}_q} \sum_{x=0,1} \sqrt{\frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w)} |i_1\rangle \\ &\quad \cdots |i_q\rangle \otimes |0\rangle^{\otimes(Q-q)} |k_1\rangle \cdots |k_q\rangle \otimes |0\rangle^{\otimes(Q-q)} |x\rangle \\ &\equiv \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sum_{i_q} \sum_{\mathbf{k}_q} \sum_{x=0,1} \sqrt{\frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w)} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle, \end{aligned} \quad (39)$$

where $|\mathbf{i}_q\rangle$ represents Q quantum registers that each has dimension M and $|\mathbf{k}_q\rangle$ represents Q quantum registers that

each has dimension K . The normalization constant is

$$s = \sum_{q=0}^Q \sum_{i_q} \sum_{\mathbf{k}_q} \sum_{x=0,1} \frac{\widetilde{\Delta t_w}^q}{2q!} \Gamma_{i_q}^{(\mathbf{k}_q)}(t_w) \equiv \sum_{q=0}^Q \frac{[\Gamma(t_w) \widetilde{\Delta t_w}]^q}{q!}, \quad (40)$$

where we have defined

$$\Gamma(t_w) \equiv \sum_{i=0}^M \sum_{k=1}^K \|D_i^{(k)}\|_{\max} e^{t_w \lambda_{(i,k)}}, \quad (41)$$

and we note that $\Gamma(t_w)$ is an upper bound on the maximum of the interaction Hamiltonian at time t_w , $\Gamma(t_w) \geq \|V(t_w)\|_{\max}$. The quantity $\Gamma(t_w)$ is related to the energy strength in a typical LCU setup [14]. In Appendix D, we provide an alternative way that uses a larger bound $\Gamma = MK \max_{k,i} \|D_i^{(k)}\|_{\max}$, which leads to an exponential saving for the state preparation. We proceed with $\Gamma(t_w)$ hereafter.

The OAA step in the LCU method requires $s \approx 2$. This leads to

$$\Gamma(t_w) \widetilde{\Delta t_w} = \Gamma(t_w) \frac{e^{\Delta t_w \lambda} - 1}{\lambda} = \ln 2, \quad (42)$$

and Eq. (40) becomes a truncated Taylor expansion of 2 up to order Q , i.e., $2 \approx \sum_{q=0}^Q (\ln 2)^q / q!$. If we require $|s - 2| \leq \epsilon/r$, where r is the total number of steps and ϵ is some positive number, then the simulation error for each $U_I(t_w + \Delta t_w, t_w)$ is also within ϵ/r . The required truncation order with this accuracy scales as

$$Q = \mathcal{O} \left(\frac{\log(r/\epsilon)}{\log \log(r/\epsilon)} \right). \quad (43)$$

1. Time partitioning and the number of time steps

The condition in Eq. (42) imposes a constraint on the next step size Δt_w given the current time t_w ,

$$\Delta t_w = \frac{1}{\lambda} \ln \left(1 + \frac{\lambda}{\Gamma(t_w)} \ln 2 \right). \quad (44)$$

Remembering that $\Gamma(t_w)$ is a function of $t_w = \sum_{l=0}^{w-1} \Delta t_l$, this condition determines the schedule, as every Δt_w is determined by the preceding time steps.

Special care should be given when setting the last time step, as Δt_w can become too large that it exceeds the total desired evolution time T . Whenever t_{w+1} is found to be greater than T [or if the argument inside the $\ln(\cdot)$ is found to be negative], one should replace the bound $\Gamma(t_w)$ with a larger bound $\tilde{\Gamma}(t_w) = \lambda \ln 2 / (e^{\lambda \Delta t_w} - 1)$ and set the final step $\Delta t_w = T - t_w$.

Let us now examine the dependence of Δt_w on $\Gamma(t_w)$ in order to determine a bound on the number of time steps (equivalently, number of repetitions) r required for the execution of the entire time evolution. We distinguish between three cases. (i) When $\lambda = 0$, we have $\Delta t_w \Gamma(t_w) = \ln 2$, similar to the time-independent case, though we note that a vanishing maximal λ could imply time-dependent oscillations as well. This can be seen by taking the $\lambda \rightarrow 0$ limit of Eq. (44). (ii) In the case where $\lambda < 0$, i.e., a system with a decaying $\Gamma(t_w)$, we have $\Delta t_w \Gamma(t_w) \geq \ln 2$, i.e., the time steps are longer than $\ln 2 / \Gamma(t_w)$. Furthermore, the total number of steps r is finite even for an arbitrarily large evolution time T . Note that, since $\Gamma(t_w)$ approaches zero asymptotically, for a large enough time t_{w*} , we have $\Gamma(t_{w*}) < |\lambda| \ln 2$, i.e., the argument inside the logarithm above becomes negative. This indicates it reaches the final step, i.e., the bound should be modified as $\tilde{\Gamma}(t_{w*}) = \lambda \ln 2 / (e^{\lambda \Delta t_{w*}} - 1)$ and $\Delta t_{w*} = T - t_{w*}$ becomes the final step. (iii) In the case where $\lambda > 0$ [an amplified $\Gamma(t_w)$], we have $\Gamma(t_w) \gg \lambda$ at large simulation times, t_w . From Eq. (44), we have $\Delta t_w \rightarrow \ln 2 / \Gamma(t_w)$ in this limit.

We see that (for large enough simulation times) the time step Δt_w is inversely proportional to $\Gamma(t_w)$ that upper bounds the max-norm of the interaction Hamiltonian at time t_w . Therefore, we have $\sum_{w=0}^{r-1} \Gamma(t_w) \Delta t_w \gtrsim r \ln 2$, which implies that $r \lesssim \sum_{w=0}^{r-1} \Gamma(t_w) \Delta t_w / \ln 2$.

It would be instructive to compare the above scaling with that of Ref. [17] in which the simulation algorithm is said to have an L^1 -norm scaling, i.e., an algorithm cost scaling linearly with $\int_0^t d\tau H_{\max}(\tau)$ up to logarithmic factors. Under a similar intuition, our algorithm has a *discretized* L^1 -norm-like scaling with $\sum_{w=0}^{r-1} \Gamma(t_w) \Delta t_w$. However, in our case, $\Gamma(t_w)$ is related to the norm of the interaction Hamiltonian.

2. State preparation

In this subsection, we provide a procedure to prepare the state $|\psi_0\rangle$ given in Eq. (39). First, we initialize a state $|0\rangle^{\otimes Q} |0\rangle^{\otimes Q} |0\rangle$, where each of the first Q registers has dimension M (responsible for the $|\mathbf{i}_q\rangle$ part), each of the later Q registers has dimension K (responsible for the $|\mathbf{k}_q\rangle$ part), and the last register is a qubit (for the cosine decomposition). For simplicity, we can perform a Hadamard gate on the last qubit and then omit its dependence for the following discussion. The next step is to create a state of the form

$$\frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{s_q} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)}, \quad (45)$$

where $s_q \equiv [\Gamma(t_w) \tilde{\Delta t_w}]^q / q!$. For each $|1\rangle$ from the first Q registers (the $|\mathbf{i}_q\rangle$ part) and the corresponding $|1\rangle$ in the

later Q registers (the $|\mathbf{k}_q\rangle$ part), we make

$$|1\rangle |1\rangle \rightarrow \sum_{i=0}^M \sum_{k=1}^K \sqrt{\frac{||D_i^{(k)}||_{\max} e^{t_w \lambda_{(i,k)}}}{\Gamma(t_w)}} |i\rangle |k\rangle. \quad (46)$$

Then Eq. (45) becomes

$$\begin{aligned} & \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{s_q} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sqrt{\frac{\Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w)}{[\Gamma(t_w)]^q}} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle \\ &= \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sqrt{\frac{(\tilde{\Delta t_w})^q}{q!} \Gamma_{\mathbf{i}_q}^{(\mathbf{k}_q)}(t_w)} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle, \end{aligned} \quad (47)$$

which is the required $|\psi_0\rangle$ in Eq. (39), when combined with $|x\rangle$.

Next, we provide a process that produces the state in Eq. (45). First, we perform a rotation that takes the first register in the $|\mathbf{i}_q\rangle$ part to

$$|0\rangle \rightarrow \frac{1}{\sqrt{s}} \left(|0\rangle + \sqrt{\sum_{q=1}^Q s_q} |1\rangle \right), \quad (48)$$

and perform a control gate from the first register to the second (both in the $|\mathbf{i}_q\rangle$ part) such that

$$\begin{aligned} & \frac{1}{\sqrt{s}} \left(|0\rangle + \sqrt{\sum_{q=1}^Q s_q} |1\rangle \right) |0\rangle \rightarrow \frac{1}{\sqrt{s}} \left[|00\rangle \right. \\ & \left. + \sqrt{\sum_{q=1}^Q s_q} |1\rangle \frac{1}{\sqrt{\sum_{q=1}^Q s_q}} \left(\sqrt{s_1} |0\rangle + \sqrt{\sum_{q=2}^Q s_q} |1\rangle \right) \right] \\ &= \frac{1}{\sqrt{s}} \left(|00\rangle + \sqrt{s_1} |10\rangle + \sqrt{\sum_{q=2}^Q s_q} |11\rangle \right). \end{aligned} \quad (49)$$

Continuing this procedure for the rest of the registers in the $|\mathbf{i}_q\rangle$ part, the state becomes

$$|0\rangle^{\otimes Q} \rightarrow \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{s_q} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)}. \quad (50)$$

At this step, we perform controlled-NOT (CNOT) operations [35] from the first Q registers ($|\mathbf{i}_q\rangle$ part) to the last Q registers ($|\mathbf{k}_q\rangle$ part) correspondingly, e.g., perform a CNOT operation from the first register in the $|\mathbf{i}_q\rangle$ part to the first register in the $|\mathbf{k}_q\rangle$ part, and so on and so forth. Finally, we

have

$$\begin{aligned} & \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{s_q} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)} |0\rangle^{\otimes Q} \\ & \rightarrow \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{s_q} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)}, \quad (51) \end{aligned}$$

which gives Eq. (45), as required. The estimated gate cost for the preparation of $|\psi_0\rangle$ is $\mathcal{O}(QMK)$. More detail regarding the cost is provided in Sec. III D 1.

3. Implementation of the controlled unitaries

The second ingredient of the LCU routine is the construction of the controlled operation

$$V_c |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle |\psi\rangle = |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle (-i)^q P_{\mathbf{i}_q} \Phi_{\mathbf{i}_q \rightarrow x}^{(\mathbf{k}_q, w)} |\psi\rangle. \quad (52)$$

Taking an approach similar to that taken in Ref. [34], we first note that Eq. (52) indicates that V_c can be carried out in two steps: a controlled-phase operation ($V_{c\Phi}$) followed by a controlled-permutation operation (V_{cP}).

The controlled-phase operation $V_{c\Phi}$ requires a somewhat intricate calculation of nontrivial phases. We therefore carry out the required algebra with the help of additional ancillary registers and then “push” the results into phases. The latter step is done by employing the unitary

$$U_{\text{ph}}|\varphi\rangle = e^{-i\varphi}|\varphi\rangle, \quad (53)$$

whose implementation cost depends only on the precision with which we specify φ and is independent of Hamiltonian parameters [33] (see Ref. [34] for a complete derivation). With the help of the (controlled) unitary transformation

$$V_{\chi\Phi} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle |z\rangle |0\rangle = |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle |z\rangle |\chi_{\mathbf{i}_q}^{(z)} + (-1)^k \phi_{\mathbf{i}_q}^{(z)}\rangle, \quad (54)$$

we can write $V_{c\Phi} = V_{\chi\Phi}^\dagger (1 \otimes U_{\text{ph}}) V_{\chi\Phi}$, so that

$$V_{c\Phi} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle |z\rangle = |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle \Phi_{\mathbf{i}_q}^{(k)} |z\rangle. \quad (55)$$

Note that $V_{\chi\Phi}$ sends computational basis states to computational basis states. We provide an explicit construction of $V_{\chi\Phi}$ in Ref. [34]. We find that its gate cost is $\mathcal{O}[QM(k_{\text{od}} + \log M) + QMK(C_D + C_{\Delta H_0} + C_\Lambda)]$ and qubit cost is $\mathcal{O}[Q \log(MK)]$. Additional details are provided in Sec. III D 1.

The construction of V_{cP} is carried out by a repeated execution of the simpler unitary transformation $U_p |i\rangle |z\rangle = |i\rangle P_i |z\rangle$. Recall that the P_i are the off-diagonal permutation operators that appear in the Hamiltonian. The gate cost of U_p is therefore $\mathcal{O}[M(k_{\text{od}} + \log M)]$. Additional details may be found in Ref. [34].

D. Algorithm cost

We next analyze the circuit costs for the permutation expansion algorithm. Recall that the simulation of $U(T)$ consists of two operations— $e^{-iH_0 T}$ and $U_I(T)$. The diagonal unitary $e^{-iH_0 T}$ can be implemented efficiently with a gate cost that scales linearly with the system size. To observe this, note that H_0 is a diagonal matrix with real diagonal elements and can be written as $H_0 = \sum_{\gamma=0}^L J_\gamma Z_\gamma$, where each Z_γ is a tensor products of Pauli-Z operators ($Z \otimes \cdots \otimes Z$) acting on at most d qubits (weight- d operators). Hence, we can write $e^{-iH_0 T} = \prod_{\gamma=0}^L e^{-iJ_\gamma Z_\gamma T}$. Each $e^{-iJ_\gamma Z_\gamma T}$ can be simulated using at most $2d$ CNOT gates with a single ancillary qubit. For example, let Z_γ be a weight- m ($m \leq d$) operator; then $e^{-iJ_\gamma Z_\gamma T}$ can be implemented as

where $|z_1\rangle \cdots |z_m\rangle$ are the qubits Z_γ acts on and $|0\rangle$ is an ancillary qubit for extracting the phase. There are total L such implementations for $e^{-iH_0 T}$. Therefore, the total gate cost is $\mathcal{O}(Ld)$ and the qubit cost is $\mathcal{O}(1)$. Since L usually grows linearly with the system size, the gate cost also scales linearly.

1. The cost for the state preparation and the controlled unitaries

The cost of implementing $U_I(T)$ resembles that in Ref. [34]. The first ingredient is the preparation of state $|\psi_0\rangle$. Recall from Sec. III C 2 that the operation that takes $|0\rangle^{\otimes Q} |0\rangle^{\otimes Q} |0\rangle$ to $(1/\sqrt{s}) \sum_{q=0}^Q \sqrt{s_q} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)}$ has gate cost $\mathcal{O}(Q)$. The operation for $|1\rangle |1\rangle \rightarrow \sum_{i=0}^M \sum_{k=1}^K \sqrt{[||D_i^{(k)}||_{\max} e^{t_w \lambda_{(i,k)}} / \Gamma(t_w)] |i\rangle |k\rangle}$ costs $\mathcal{O}(MK)$ [14,36]. The total gate cost for the preparation of $|\psi_0\rangle$ (i.e., B) is $\mathcal{O}(QMK)$. In Appendix D, we provide an alternative procedure that leads to a $\mathcal{O}[Q \log(MK)]$ scaling for implementing B . The qubit cost in the state preparation is $\mathcal{O}[Q \log(MK)]$.

The next component is the implementation of the control unitary V_c . As shown in Ref. [34], the gate cost of performing the control permutation $P_{\mathbf{i}_q}$ is $\mathcal{O}[QM(k_{\text{od}} + \log M)]$, where k_{od} is the “locality,” i.e., each permutation P_i is a tensor product of at most k_{od} Pauli- X operators. The implementation of the control phase $\Phi_{\mathbf{i}_q \rightarrow x}^{(\mathbf{k}_q, w)}$ involves the calculation of $d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)}$ (the product of diagonal elements in the permutation expansion) and the divided differences (with the x_j being the inputs). The cost of the former is $\mathcal{O}(QMKC_D)$, where C_D is the cost of obtaining an

element of $D_i^{(k)}$. The cost of the latter is $\mathcal{O}[QM(k_{\text{od}} + \log M) + QMK(C_{\Delta H_0} + C_\Lambda)]$, where $C_{\Delta H_0}$ (C_Λ) is the cost of obtaining energy differences of H_0 (elements of $\Lambda_i^{(k)}$) [therefore, $C_{\Delta H_0} + C_\Lambda$ is the cost for obtaining the inputs, x_j , as defined in Eq. (28)]. The additional cost for the reversibility of the process scales as $\mathcal{O}(Q^2)$. A detailed discussion of the costs of $C_{\Delta H_0}$ and C_Λ may be found in Ref. [34]. Combining these, we estimate that the total cost for V_c is

$$\mathcal{O}[Q^2 + QM(k_{\text{od}} + \log M) + QMK(C_D + C_{\Delta H_0} + C_\Lambda)]. \quad (56)$$

2. Overall cost of the algorithm

The full simulation for $U_I(T)$ is a product of segments $U_I(t_w + \Delta t_w, t_w)$, where each segment is simulated by interleaving B and V_c . The total number of segments, r , is determined by $T = \sum_{w=0}^{r-1} \Delta t_w$, where each Δt_w is determined by the partitioning scheme described in Sec. III C 1.

As discussed above, the number of LCU applications r can be upper bounded by $r \lesssim \sum_{w=0}^{r-1} \Gamma(t_w) \Delta t_w / \ln 2$ (in the long simulation time limit), which can be viewed as a discretized L^1 -norm-like scaling with the norm of the nonstatic component of the Hamiltonian $V(t)$.

Combining with the cost for simulating $e^{-iH_0 T}$ with the cost for each step (56), we conclude that at worst the total gate cost scales as

$$\mathcal{O}[rQ^2 + rQM(k_{\text{od}} + \log M) + rQMK(C_D + C_{\Delta H_0} + C_\Lambda) + Ld], \quad (57)$$

and the qubit cost scales as

$$\mathcal{O}[Q \log(MK)], \quad (58)$$

where Q scales as $\mathcal{O}[\log(r/\epsilon)/\log \log(r/\epsilon)]$. A summary of the gate and qubit costs of the simulation circuit and the various subroutines used to construct it is given in Table I. A comparison to the best existing algorithms is also provided in Table II.

3. Example advantages of the algorithm

To illustrate how our simulation algorithm can provide speedups over existing algorithms, we focus in this subsection on two types of Hamiltonian system: highly oscillating systems and decaying systems.

The cost of our algorithm is independent of the oscillation rates of the dynamics, whereas the cost of any simulation algorithm (e.g., Refs. [12, 15–17]) that depends on $\|dH(t)/dt\|$ would depend on oscillation rates of the system. To illustrate this advantage, consider a two-level

system with a Hamiltonian

$$H(t) = hZ + \Gamma(e^{-i\alpha t}|0\rangle\langle 1| + e^{i\alpha t}|1\rangle\langle 0|) = H_0 + V(t), \quad (59)$$

where $h, \Gamma, \alpha \in \mathbb{R}$, $H_0 = hZ$, and $V(t) = \Gamma(e^{-i\alpha t}|0\rangle\langle 1| + e^{i\alpha t}|1\rangle\langle 0|)$. In this case, we have $k_{\text{od}} = M = K = 1$ and $\lambda = 0$. The gate cost of simulating $U(T)$ scales as

$$\mathcal{O}\left[\Gamma T \left(\frac{\log \Gamma T / \epsilon}{\log \log \Gamma T / \epsilon}\right)^2\right], \quad (60)$$

which is independent of α . This means that the simulation cost remains the same even if α becomes arbitrarily large. One can realize the absence of α owing to the fact that phases are explicitly integrated out into an integral-free expansion series, where the bound of each term does not depend on the oscillations (see Identity 2). Therefore, our simulation can be significantly more effective when the time dependence of the Hamiltonian has very high frequencies. Note that while the example above was given for a simple qubit system with pure oscillation, the frequency independence in cost holds for any system.

Another class of systems for which our algorithm can provide speedup are Hamiltonians with exponential decays, i.e., $\lambda < 0$, which play an important role in many-body physics [37]. For concreteness, consider the Hamiltonian

$$H(t) = hZ + \Gamma e^{-\alpha t} X = H_0 + V(t), \quad (61)$$

where $h, \Gamma \in \mathbb{R}$, $\alpha > 0$, $H_0 = hZ$, and $V(t) = \Gamma e^{-\alpha t} X$. In this case, $\lambda = -\alpha$ and $\|V(t)\|_{\max} = \Gamma e^{-\alpha t}$.

The L^1 -norm defined in Ref. [17] is $\int_0^T \|H(t)\|_{\max} dt$, which has a linear scaling $\mathcal{O}(hT)$ with the simulation duration T , whereas our discretized L^1 -norm $\sum_{w=0}^{r-1} \|V(t_w)\|_{\max} \Delta t_w$ tends to a constant in the long time limit. This can be seen from the fact that the partition terminates at a large enough time t_w ($\leq T$), where $\Delta t_w = T - t_w$ becomes the final simulation step, as described in Sec. III C 1. The above results also hold for any combination of exponential decays (even when these are multiplied by oscillatory terms) with which different time decay dependencies may be constructed.

E. Hamiltonians with arbitrary time dependence

The simulation algorithm invokes a switch to the interaction picture, by dividing the Hamiltonian into a static diagonal part H_0 and a time-dependent Hermitian operator $V(t)$. The $V(t)$ is expanded using permutations and exponential sums as presented in Eq. (16). There, we assume that the time dependence can be expressed as exponential sums with a finite number of terms, K . Although this assumption holds for many models (e.g., when the

TABLE I. A summary of resources for the circuit.

Unitary	Gate cost	Qubit cost
e^{-iH_0T}	$\mathcal{O}(Ld)$	$\mathcal{O}(1)$
V_c	$\mathcal{O}[Q^2 + QM(k_{\text{od}} + \log M) + QMK(C_D + C_{\Delta H_0} + C_\Lambda)]$	$\mathcal{O}(Q \log MK)$
$U_I(T)$	$\mathcal{O}\{r[Q^2 + QM(k_{\text{od}} + \log M) + QMK(C_D + C_{\Delta H_0} + C_\Lambda)]\}$	$\mathcal{O}(Q \log MK)$

time dependencies are some combinations of trigonometric functions and exponential decays), the exponential series generally requires an infinite sum (e.g., a Fourier series). A straightforward procedure to obtain a finite sum approximation is via a truncated Fourier series. As an example, let us consider a polynomial function of time, i.e., $f(t) = \sum_{l=0}^p c_l t^l$. Using the proof of Theorem 8.14 in Ref. [38], it can be shown that a truncated Fourier series of $f(t)$ is $\mathcal{O}(\epsilon)$ close to $f(t)$ when the truncation order is $\mathcal{O}(1/\epsilon)$. We also note that, other than the Fourier series, there have been numerous studies [27–31] regarding finding an exponential-sum approximation of a function. Some of them, e.g., Ref. [27], provide efficient algorithms with logarithmically scaling terms (with respect to the inverse of a required accuracy). These results suggest that efficient methods for finding the exponential-sum decompositions of the time dependencies of $V(t)$ can exist in many cases.

Suppose that $V(t)$ is approximated by a finite series of an exponential sum. The resulting error of the unitary evolution, due to the Hamiltonian approximation, scales only at most linearly with the evolution duration. This can be shown using the following property. Given two time-dependent Hamiltonians $H_1(t)$ and $H_2(t)$ such that

$$\|H_1(t) - H_2(t)\| \leq \epsilon \quad \text{for all } t \in [0, T], \quad (62)$$

then

$$\begin{aligned} \|U_1(T, 0) - U_2(T, 0)\| &\equiv \left\| \mathcal{T} \exp \left[-i \int_0^T H_1(t) dt \right] \right. \\ &\quad \left. - \mathcal{T} \exp \left[-i \int_0^T H_2(t) dt \right] \right\| \\ &\leq \epsilon T. \end{aligned} \quad (63)$$

This holds for any norm $\|\cdot\|$. Before proving this, we first note a property of the so-called subadditivity of error

in implementing unitaries [33]. It says that, for unitaries U_1, U_2, V_3 , and V_4 , we have

$$\|U_2 U_1 - V_2 V_1\| \leq \|U_2 - V_2\| + \|U_1 - V_1\|. \quad (64)$$

This can be easily shown by

$$\begin{aligned} \|U_2 U_1 - V_2 V_1\| &= \|U_2 U_1 - V_2 U_1 + V_2 U_1 - V_2 V_1\| \\ &\leq \|(U_2 - V_2) U_1\| + \|V_2 (U_1 - V_1)\| \\ &\leq \|U_2 - V_2\| + \|U_1 - V_1\|, \end{aligned} \quad (65)$$

where the basic operator norm inequalities are used. Now we prove the bound in Eq. (63). We divide T into n segments such that each segment has width T/n . We can rewrite the time evolution operators as

$$\begin{aligned} U_1(T, 0) &= U_1 \left(T, \frac{n-1}{n} T \right) \cdots U_1 \left(\frac{T}{n}, 0 \right), \\ U_2(T, 0) &= U_2 \left(T, \frac{n-1}{n} T \right) \cdots U_2 \left(\frac{T}{n}, 0 \right). \end{aligned}$$

Repeatedly using the subadditivity of error, we have

$$\begin{aligned} \|U_1(T, 0) - U_2(T, 0)\| &\leq \sum_{m=1}^n \left\| U_1 \left(\frac{mT}{n}, \frac{(m-1)T}{n} \right) - U_2 \left(\frac{mT}{n}, \frac{(m-1)T}{n} \right) \right\| \\ &\leq \sum_{m=1}^n \left\| \int_{(m-1)T/n}^{mT/n} [H_1(t) - H_2(t)] dt \right\| + \sum_{m=1}^n \mathcal{O} \left[\left(\frac{T}{n} \right)^2 \right] \\ &\leq \sum_{m=1}^n \epsilon \frac{T}{n} + \sum_{m=1}^n \mathcal{O} \left[\left(\frac{T}{n} \right)^2 \right] \\ &= \epsilon T + \mathcal{O} \left[\frac{T^2}{n} \right]. \end{aligned} \quad (66)$$

TABLE II. A comparison of gate costs with the best existing algorithms. Both approaches in Ref. [17] have $H(t) = \sum_{\ell=1}^{L'} \alpha_\ell(t) H_\ell$, where the H_ℓ are some unitary operators and $\alpha(t)$ some time-dependent coefficients. Here $\|\alpha\|_{1,1} \equiv \sum_{\ell=1}^{L'} \int_0^T dt \alpha_\ell(t) \|H_\ell\|_\infty$, $\|\alpha\|_{\infty,1} \equiv \int_0^T dt \|\alpha_\ell(t)\|_\infty$, g_c is the gate cost for implementing each controlled H_ℓ , and g_e is the gate cost for each controlled $e^{-iH_\ell t}$.

Algorithms	Gate complexity
Continuous qDRIFT in Ref. [17]	$\mathcal{O}(\ \alpha\ _{1,1}^2 g_e / \epsilon)$
Rescaled Dyson series in Ref. [17]	$\tilde{\mathcal{O}}(\ \alpha\ _{\infty,1} L^2 g_c)$
This paper	$\mathcal{O}\{r[Q^2 + QM(k_{\text{od}} + \log M) + QMK(C_D + C_{\Delta H_0} + C_\Lambda)] + Ld\}$

Since this inequality holds for any n , we can take $n \rightarrow \infty$ and it yields Eq. (63) as claimed.

Now we apply this property to the simulation of $U_I(T)$. Suppose that we have a $\tilde{\delta}$ -accurate approximation of $V(t)$, i.e., $\|\tilde{V}(t) - V(t)\| \leq \tilde{\delta}$ for all $t \in [0, T]$, where $\tilde{V}(t)$ is the finite exponential-sum approximation of $V(t)$. The accumulative error from this approximation is bounded by $\tilde{\delta}T$ and the overall error is $\mathcal{O}(\tilde{\delta}T + \delta)$, where δ is the error from the LCU implementation. Recall that $\tilde{\delta}$ is closely related to K (the number of terms). Although it is intuitive that a larger K can allow for a smaller δ , the explicit relation between the two largely depends on the model and the expansion method. Nonetheless, we can expect K to scale at least linearly with $1/\tilde{\delta}$ for many cases, e.g., the aforementioned truncated Fourier series for a polynomial.

The simulation cost also depends on M , the number of terms in the permutation expansion. This quantity usually scales linearly with the system size and can be easily determined. For example, a typical spin model usually involves a sum of tensor products of Pauli- X (or Y) operators and Pauli- Z . Each tensor product represents an interaction between qubits on certain lattice sites. Because of the common locality constraint that prevents a qubit interacting with those arbitrarily far apart, the number of interacting terms, M , scales at most linearly with the number of qubits. In addition, a tensor product of Pauli operators can be easily separated into a product of diagonal matrices and a permutation, e.g., $X \otimes X \otimes Y = (I \otimes I \otimes -iZ)(X \otimes X \otimes X)$. We conclude that M will have modest linear scaling for most practical models.

IV. ALTERNATIVE SCHEME AND REDUCTION TO THE TIME-INDEPENDENT CASE

In this section, we provide an alternative yet equivalent scheme for the dynamical simulation, one that will allow us to establish an immediate connection to the time-independent Hamiltonian simulation formalism (specifically to the scheme presented in Ref. [34]), in which $H(t)$ is assumed constant in time.

In previous sections, we have chosen to partition the interaction-picture unitary $U_I(T)$ into short time segments and then follow its execution by the application of a diagonal e^{iH_0T} , bringing it back to the Schrödinger picture. Here, we show that the Schrödinger picture $U(T)$ can be partitioned similarly.

Recalling the expansion of $U_I(t_w + \Delta t_w, t_w)$ in Eq. (31), we have

$$\begin{aligned} U_I(t_w + \Delta t_w, t_w)|z\rangle \\ = \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{t_w x_1} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \end{aligned}$$

with

$$x_1 = i(E_{z_{\mathbf{i}_q}} - E_z) + \sum_{l=1}^q \lambda_{i_l, z_{\mathbf{i}_l}}^{(k_l)}.$$

Breaking the $e^{t_w x_1}$ phase, we get

$$\begin{aligned} U_I(t_w + \Delta t_w, t_w)|z\rangle \\ = \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{t_w \sum_{l=1}^q \lambda_{i_l, z_{\mathbf{i}_l}}^{(k_l)}} e^{-it_w E_z} e^{i(t_w + \Delta t_w) E_{z_{\mathbf{i}_q}}} \\ \times e^{-i\Delta t_w E_{z_{\mathbf{i}_q}}} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle. \end{aligned} \quad (67)$$

We find that

$$e^{-iH_0(t_w + \Delta t_w)} U_I(t_w + \Delta t_w, t_w) = \tilde{U}_I(t_w + \Delta t_w, t_w) e^{-iH_0 t_w},$$

where

$$\begin{aligned} \tilde{U}_I(t_w + \Delta t_w, t_w) \\ = \sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{t_w \sum_{l=1}^q \lambda_{i_l, z_{\mathbf{i}_l}}^{(k_l)}} \\ \times e^{-i\Delta t_w E_{z_{\mathbf{i}_q}}} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \langle z|. \end{aligned} \quad (68)$$

Inspecting the full unitary evolution, we observe that

$$\begin{aligned} U(T) &= e^{-iH_0T} U_I(T) \\ &= e^{-iH_0T} U_I(T, t_{r-1}) U_I(t_{r-1}, t_{r-2}) \cdots U_I(t_1, 0) \\ &= \tilde{U}_I(T, t_{r-1}) D(t_{r-1}) U_I(t_{r-1}, t_{r-2}) \cdots U_I(t_1, 0). \end{aligned} \quad (69)$$

The evolution operator $U(T)$ can be simplified as

$$U(T) = \tilde{U}_I(T, t_{r-1}) \tilde{U}_I(t_{r-1}, t_{r-2}) \cdots \tilde{U}_I(t_1, 0), \quad (70)$$

eliminating the diagonal piece. Each $\tilde{U}_I(t_w + \Delta t_w, t_w)$ can be rewritten as

$$\begin{aligned} \tilde{U}_I(t_w + \Delta t_w, t_w) \\ = \sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{(t_w + \Delta t_w) \sum_{l=1}^q \lambda_{i_l, z_{\mathbf{i}_l}}^{(k_l)}} \\ \times e^{-\Delta t_w (iE_{z_{\mathbf{i}_q}} + \sum_{l=1}^q \lambda_{i_l, z_{\mathbf{i}_l}}^{(k_l)})} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \langle z|. \end{aligned} \quad (71)$$

The factor $e^{-\Delta t_w(iE_{z_{i_q}} + \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)})}$ can be absorbed into the divided difference

$$\begin{aligned} \tilde{U}_I(t_w + \Delta t_w, t_w) &= \sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{(t_w + \Delta t_w) \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)}} \\ &\quad \times e^{\Delta t_w [\tilde{y}_1, \tilde{y}_2, \dots, \tilde{y}_q, \tilde{y}_{q+1}]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \langle z| \end{aligned} \quad (72)$$

with

$$\begin{aligned} \tilde{y}_j &= x_j - \left(iE_{z_{i_q}} + \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)} \right) \\ &= i(E_{z_{i_q}} - E_{z_{i_{j-1}}}) + \sum_{l=j}^q \lambda_{i_l, z_{i_l}}^{(k_l)} - \left(iE_{z_{i_q}} + \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)} \right), \end{aligned}$$

which simplifies to

$$\tilde{y}_j = -iE_{z_{i_{j-1}}} - \sum_{l=1}^{j-1} \lambda_{i_l, z_{i_l}}^{(k_l)}. \quad (73)$$

By inserting additional $i\Delta t_w E_z$ phases into the divided differences, we can rewrite

$$\begin{aligned} \tilde{U}_I(t_w + \Delta t_w, t_w) &= \left(\sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q e^{(t_w + \Delta t_w) \sum_{l=1}^q \lambda_{i_l, z_{i_l}}^{(k_l)}} \right. \\ &\quad \times e^{\Delta t_w [y_1, y_2, \dots, y_q, y_{q+1}]} d_{\mathbf{i}_q, z}^{(\mathbf{k}_q)} P_{\mathbf{i}_q} |z\rangle \langle z| \Big) \\ &\quad \times e^{-iH_0 \Delta t_w} \end{aligned} \quad (74)$$

with

$$\begin{aligned} y_j &= \tilde{y}_j + iE_z = -i(E_{z_{i_{j-1}}} - E_z) - \sum_{l=1}^{j-1} \lambda_{i_l, z_{i_l}}^{(k_l)} \\ &= -i\Delta E_{z_{i_{j-1}}} - \sum_{l=1}^{j-1} \lambda_{i_l, z_{i_l}}^{(k_l)}. \end{aligned}$$

Now, we can write $U(T)$ as alternating off-diagonal and diagonal unitaries:

$$\begin{aligned} U(T) &= \prod_w \tilde{U}_I(t_w + \Delta t_w, t_w) \\ &\equiv \prod_w U_{\text{od}}(t_w + \Delta t_w, t_w) e^{-iH_0 \Delta t_w}. \end{aligned} \quad (75)$$

When $H(t)$ becomes time independent, $\lambda_{i_l, z_{i_l}}^{(k_l)} = 0$ and $\Delta t_w = \Delta t = \ln 2 / \Gamma$. To synchronize the notation with that of Ref. [34], we identify $H_0 = D_0$ and $U_{\text{od}}(t_w + \Delta t_w, t_w) = U_{\text{od}}$. The evolution operator becomes $U(T) = U_{\text{od}} e^{-iD_0 \Delta t} \dots U_{\text{od}} e^{-iD_0 \Delta t}$, which coincides with Ref. [34].

V. CONCLUSIONS

We have presented a quantum algorithm for simulating the evolution operator generated from a time-dependent Hamiltonian. The algorithm involves a permutation expansion for the interaction Hamiltonian, a switch to the interaction picture, and the incorporation of the LCU technique. Combining the permutation expansion with the Dyson series leads to an integral-free representation for the interaction-picture unitary with coefficients involving the notion of divided differences with complex inputs.

We find that our expansion allows us to adjust the time steps based on the dynamical characteristics of the Hamiltonian, providing a resource saving as compared to the equal-size partition with the largest bound. This further results in a gate resource that scales with an L^1 -norm-like scaling with respect only to the “nonstatic” norm of the Hamiltonian. Our expansion also improves on the traditional product-formula algorithms, where the evolution operator is divided into equal-size pieces, where each piece is approximated by a time-independent Hamiltonian simulation, i.e., $e^{-iH_l \Delta t}$.

Specifically, we have demonstrated that, for systems with a decaying nonstatic component, the resources do not scale with the total evolution time asymptotically. Furthermore, the simulation cost is independent of the frequencies, implying a significant advantage for systems with highly oscillating components.

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APPENDIX A: PROPERTIES OF DIVIDED DIFFERENCE

We begin with a formal definition of divided difference for complex-valued functions and follow with some properties that will be of use to us when deriving the new bound. The main results are derived for the exponential functions.

Definition 1. Let $\mathbb{U}$ be an open subset of $\mathbb{C}$, and $f : \mathbb{U} \rightarrow \mathbb{C}$ is analytic in $\mathbb{U}$. For any non-negative integer q and $x_0, x_1, \dots, x_q \in \mathbb{U}$, the divided difference of f is denoted as $f[x_0, x_1, \dots, x_q]$. If $q = 0$, $f[x_0] \equiv f(x_0)$. Suppose that $\{x_0, x_1, \dots, x_q\}$ has r distinct elements. Let $S = \{x_{\sigma(0)}, x_{\sigma(1)}, \dots, x_{\sigma(q)}\}$ be a sorted set of $\{x_0, x_1, \dots, x_q\}$, i.e., there exists a permutation σ such that the first n_1 elements of S are equal and the following n_2 elements of S are equal, and so on and so forth. There are r same-element clusters and $\sum_{i=1}^r n_i = q + 1$. The divided difference of f

is defined as

$$f[x_0, x_1, \dots, x_q] = \begin{cases} \frac{f[x_{\sigma(1)}, \dots, x_{\sigma(q)}] - f[x_{\sigma(0)}, \dots, x_{\sigma(q-1)}]}{x_{\sigma(q)} - x_{\sigma(0)}} & \text{if } r > 1, \\ \frac{f^{(q)}(x_0)}{q!} & \text{if } r = 1, \end{cases} \quad (\text{A1})$$

where $f^{(q)}$ denotes the q th derivative of f .

Although the above sorting procedure is not unique, it can be shown that any choice of the permutation gives the same result, and hence the definition is well defined.

The divided difference involves a recursive relation that connects a $q + 1$ input case to two q cases. For $q = 1$,

$$f[x_0, x_1] = \begin{cases} \frac{f(x_1) - f(x_0)}{x_1 - x_0} & \text{if } x_0 \neq x_1, \\ f'(x_0) & \text{if } x_0 = x_1. \end{cases} \quad (\text{A2})$$

For $q = 2$, and suppose x_0, x_1 and x_2 are all distinct,

$$\begin{aligned} f[x_0, x_1, x_2] &= \frac{1}{x_2 - x_0} \left(\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0} \right) \\ &= \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_2)(x_1 - x_0)} \\ &\quad + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}. \end{aligned} \quad (\text{A3})$$

In fact, it can be shown that, for distinct $x_0, x_1, \dots, x_q$,

$$f[x_0, x_1, \dots, x_q] = \sum_{i=0}^q \frac{f(x_i)}{\prod_{k \neq i} (x_i - x_k)}. \quad (\text{A4})$$

Remark. Since any analytic function admits a Taylor expansion representation and the divided difference is a linear functional, the divided difference of an analytic function f has a series expansion form, i.e., for $x_0, \dots, x_q$ and y in f 's analytic domain,

$$f[x_0, \dots, x_q] = \sum_{n=0}^{\infty} \frac{f^{(n)}(y)}{n!} p_{n|y}[x_0, \dots, x_q], \quad (\text{A5})$$

where $p_{n|y}(x) \equiv (x - y)^n$. Because $p_{n|y}[x_0, \dots, x_q] = 0$ for all $n < q$, the nonvanishing term of the series starts from the q th order.

For simplicity, we denote the divided difference for the exponential function as $e^{[x_0, \dots, x_q]}$, i.e.,

$$e^{[x_0, \dots, x_q]} \equiv f[x_0, \dots, x_q], \quad \text{where } f(x) = e^x. \quad (\text{A6})$$

Property 1. For any non-negative integer q and $x_0, x_1, \dots, x_q \in \mathbb{C}$,

$$e^{[x_0, x_1, \dots, x_q]} = e^{x_0} e^{[0, x_1 - x_0, \dots, x_q - x_0]}. \quad (\text{A7})$$

This property and the fact that divided differences are permutation symmetric among inputs imply that any input can be factored out of the divided difference by subtracting it from every entry.

Property 2. For any non-negative integer q and $x_0, x_1, \dots, x_q \in \mathbb{C}$,

$$e^{[x_0, x_1, \dots, x_q]} = \sum_{n=q}^{\infty} \frac{1}{n!} \sum_{\sum k_j = n-q} \prod_{j=0}^q (x_j)^{k_j}. \quad (\text{A8})$$

An equivalent definition of the divided difference for an analytic function is via its Taylor expansion. It amounts to applying the divided difference on every order of the series. Since any polynomial of order less than q is annihilated, the series starts from the order q . Property 2 is derived from the Taylor expansion of e^x with respect to the origin.

Lemma 1. For any non-negative integer q and $x_0, x_1, \dots, x_q \in \mathbb{C}$,

$$\int_0^1 a^q e^{[ax_0, ax_1, \dots, ax_q]} da = e^{[0, x_0, x_1, \dots, x_q]}. \quad (\text{A9})$$

Proof. This can be observed from the series expansion of the divided difference for the exponential function, i.e., from Property 2,

$$\begin{aligned} a^q e^{[ax_0, ax_1, \dots, ax_q]} &= a^q \sum_{n=q}^{\infty} \frac{1}{n!} \sum_{\sum k_j = n-q} \prod_{j=0}^q (ax_j)^{k_j} \\ &= a^q \sum_{n=q}^{\infty} \frac{1}{n!} \sum_{\sum k_j = n-q} a^{n-q} \prod_{j=0}^q (x_j)^{k_j} \\ &= \sum_{n=q}^{\infty} \frac{a^n}{n!} \sum_{\sum k_j = n-q} \prod_{j=0}^q (x_j)^{k_j}. \end{aligned} \quad (\text{A10})$$

Performing term-by-term integration over a on both sides, we have

$$\begin{aligned} \int_0^1 a^q e^{[ax_0, ax_1, \dots, ax_q]} da &= \sum_{n=q}^{\infty} \left(\int_0^1 \frac{a^n}{n!} da \right) \sum_{\sum k_j = n-q} \prod_{j=0}^q (x_j)^{k_j} \\ &= \sum_{n=q}^{\infty} \frac{1}{(n+1)!} \sum_{\sum k_j = n-q} \prod_{j=0}^q (x_j)^{k_j} \\ &= e^{[0, x_0, x_1, \dots, x_q]}, \end{aligned} \quad (\text{A11})$$

where the last equality follows from the series expansion representation of $e^{[0, x_0, x_1, \dots, x_q]}$. This completes the proof. ■

Corollary 1. Let $f(x) = e^{tx}$, where $t \in \mathbb{R}$ and $x \in \mathbb{C}$. We let $e^{t[x_0, \dots, x_q]} \equiv f[x_0, \dots, x_q]$, where $x_0, \dots, x_q \in \mathbb{C}$. For any $\tau \in \mathbb{R}$,

$$\int_0^\tau e^{t[x_0, \dots, x_q]} dt = e^{\tau[x_0, \dots, x_q]}. \quad (\text{A12})$$

This can be verified by evaluating the series expansion form on both sides, by a similar manner as in the proof of Lemma 1.

With these properties, we are ready to prove the bound in Identity 2 in the main text.

Theorem 1. For any non-negative integer q and $x_0, x_1, \dots, x_q \in \mathbb{C}$,

$$|e^{[x_0, \dots, x_q]}| \leq e^{[\text{Re}(x_0), \text{Re}(x_1), \dots, \text{Re}(x_q)]}, \quad (\text{A13})$$

where $\text{Re}(\cdot)$ gives the real part of the input.

Proof. We proceed by induction. Equation (A13) is trivially satisfied with the equality when $q = 0$. For the case $q = 1$, we have

$$\begin{aligned} |e^{[x_0, x_1]}| &= |e^{x_0}| |e^{[0, x_1 - x_0]}| \\ &= e^{\text{Re}(x_0)} \left| \int_0^1 a e^{a(x_1 - x_0)} da \right| \\ &\leq e^{\text{Re}(x_0)} \int_0^1 |a e^{a(x_1 - x_0)}| da \\ &= e^{\text{Re}(x_0)} \int_0^1 a e^{a \text{Re}(x_1 - x_0)} da \\ &= e^{[\text{Re}(x_0), \text{Re}(x_1)]}, \end{aligned} \quad (\text{A14})$$

where Lemma 1 has been used. Assume that we have

$$|e^{[x_0, \dots, x_q]}| \leq e^{[\text{Re}(x_0), \dots, \text{Re}(x_q)]}, \quad (\text{A15})$$

which is true for $q = 0, 1$. It follows that

$$|e^{[x_0, \dots, x_q, x_{q+1}]}| \quad (\text{A16})$$

$$\begin{aligned} &= |e^{x_{q+1}}| |e^{[0, x_0 - x_{q+1}, \dots, x_q - x_{q+1}]}| \\ &= e^{\text{Re}(x_{q+1})} \left| \int_0^1 a^q e^{[a(x_0 - x_{q+1}), \dots, a(x_q - x_{q+1})]} da \right| \\ &\leq e^{\text{Re}(x_{q+1})} \int_0^1 a^q |e^{[a(x_0 - x_{q+1}), \dots, a(x_q - x_{q+1})]}| da \\ &\leq e^{\text{Re}(x_{q+1})} \int_0^1 a^q e^{[\text{Re}(ax_0 - ax_{q+1}), \dots, \text{Re}(ax_q - ax_{q+1})]} da \\ &= e^{\text{Re}(x_{q+1})} e^{[0, \text{Re}(x_0 - x_{q+1}), \dots, \text{Re}(x_q - x_{q+1})]} \\ &= e^{[\text{Re}(x_0), \dots, \text{Re}(x_q), \text{Re}(x_{q+1})]}, \end{aligned} \quad (\text{A17})$$

where the second and third equalities use Lemma 1 and the second inequality uses Eq. (A15). This proves that the inequality holds for any number of complex inputs. ■

APPENDIX B: BOUNDING $|e^{\Delta t_w[x_1, x_2, \dots, x_q, 0]}|$

For $|e^{\Delta t_w[x_1, x_2, \dots, x_q, 0]}|$, we use the following theorem.

Theorem 2. For any $q + 1$ complex values $x_0, \dots, x_q \in \mathbb{C}$,

$$|e^{[x_0, \dots, x_q]}| \leq e^{[\text{Re}(x_0), \dots, \text{Re}(x_q)]}, \quad (\text{B1})$$

where $\text{Re}(\cdot)$ gives the real part of the input.

This is proved in Appendix A. From this, we have

$$\begin{aligned} |e^{\Delta t_w[x_1, \dots, x_q, 0]}| &= (\Delta t_w)^q |e^{[\Delta t_w x_1, \dots, \Delta t_w x_q, 0]}| \\ &\leq (\Delta t_w)^q e^{[\Delta t_w \text{Re}(x_1), \dots, \Delta t_w \text{Re}(x_q), 0]}. \end{aligned} \quad (\text{B2})$$

From the definition of x_j , we have, for all $j \in \{1, \dots, q\}$,

$$\text{Re}(x_j) = \sum_{l=j}^q \text{Re}(\lambda_{i_l, z_{i_l}}^{(k_l)}) \leq (q - j + 1)\lambda. \quad (\text{B3})$$

Based on the property that increasing any input in $e^{[\dots]}$ will only increase its value (which can be proved by taking derivatives in the Hermite-Genocchi form), we have

$$\begin{aligned} |e^{\Delta t_w[x_1, \dots, x_q, 0]}| &\leq (\Delta t_w)^q e^{[\Delta t_w \text{Re}(x_1), \dots, \Delta t_w \text{Re}(x_q), 0]} \\ &\leq (\Delta t_w)^q e^{[\Delta t_w q \lambda, \Delta t_w (q-1)\lambda, \dots, \Delta t_w \lambda, 0]}. \end{aligned} \quad (\text{B4})$$

Using the permutation symmetric property and Property 1, we have

$$\begin{aligned} &(\Delta t_w)^q e^{[\Delta t_w q \lambda, \Delta t_w (q-1)\lambda, \dots, \Delta t_w \lambda, 0]} \\ &= \Delta t_w^q \frac{e^{[\Delta t_w q \lambda, \Delta t_w (q-1)\lambda, \dots, \Delta t_w \lambda]} - e^{[\Delta t_w (q-1)\lambda, \dots, \Delta t_w \lambda, 0]}}{\Delta t_w \lambda q} \\ &= (\Delta t_w)^q \frac{e^{\Delta t_w \lambda} - 1}{\Delta t_w \lambda q} e^{[\Delta t_w (q-1)\lambda, \dots, \Delta t_w \lambda, 0]} \\ &= \dots \\ &= \left(\frac{e^{\lambda \Delta t_w} - 1}{\lambda} \right)^q \frac{1}{q!}. \end{aligned} \quad (\text{B5})$$

Therefore, we have

$$|e^{\Delta t_w[x_1, x_2, \dots, x_q, 0]}| \leq \frac{1}{q!} \left(\frac{e^{\lambda \Delta t_w} - 1}{\lambda} \right)^q. \quad (\text{B6})$$

APPENDIX C: LCU METHOD REVIEW

We give a brief introduction to the LCU method in this section, and we adapt the notation of the original paper [14] for a more convenient reference to readers. Suppose that we have a unitary U , which is an infinite sum of unitaries, i.e.,

$$U = \sum_{j=0}^{\infty} \beta_j V_j, \quad (C1)$$

where $\beta_j > 0$ and the V_j are some unitaries. A truncated series, up to order $m-1$, yields an operator

$$\tilde{U} = \sum_{j=0}^{m-1} \beta_j V_j, \quad (C2)$$

which approaches U as m increases. We perform the following procedure to effectively implement $\tilde{U}$ on a state $|\psi\rangle$ embedded in a larger system. Prepare an m -dimensional ancilla $|0\rangle$ and implement a unitary B such that

$$B|0\rangle = \frac{1}{\sqrt{s}} \sum_{j=0}^{m-1} \sqrt{\beta_j} |j\rangle, \quad (C3)$$

where $s = \sum_{j=0}^{m-1} \beta_j$. Suppose that we have access to a control unitary V_c such that, for each j ,

$$V_c |j\rangle |\psi\rangle = |j\rangle V_j |\psi\rangle. \quad (C4)$$

Consider the following combination of the above operations:

$$W \equiv (B^\dagger \otimes I) V_c (B \otimes I). \quad (C5)$$

We have

$$W|0\rangle |\psi\rangle = \frac{1}{s} |0\rangle \tilde{U} |\psi\rangle + \sqrt{1 - \frac{1}{s^2}} |\Phi\rangle, \quad (C6)$$

where $|\Phi\rangle$'s ancillary part is orthogonal to $|0\rangle\langle 0|$. Let us denote by $P \equiv |0\rangle\langle 0| \otimes I$ the orthogonal projection onto that subspace and by $R \equiv I - 2P$ the reflection operator with respect to P . It is shown that the sequence of operations $A \equiv -WRW^\dagger RW$ acting on the total system is $A|0\rangle |\psi\rangle = |0\rangle \tilde{U} |\psi\rangle$ when $\tilde{U}$ is unitary and $s = 2$. This procedure is the so-called oblivious amplitude amplification. However, $\tilde{U}$ is in general not unitary because it is a truncated series of U . This nonunitarity can be accounted for when $\tilde{U} \approx U$ and $s \approx 2$. More specifically, it is shown that if $\|U - \tilde{U}\| = \mathcal{O}(\delta)$ and $|s - 2| = \mathcal{O}(\delta)$ then

$$\|PA|0\rangle |\psi\rangle - |0\rangle U |\psi\rangle\| = \mathcal{O}(\delta). \quad (C7)$$

This means that, when $\tilde{U}$ is δ close to U and s is δ close to 2, the effect of the operator A on the whole system is δ close to only U acting on $|\psi\rangle$.

Note that the condition $\|U - \tilde{U}\| = \mathcal{O}(\delta)$ can be satisfied when the truncation order m is high enough. However, the condition $|s - 2| = \mathcal{O}(\delta)$ is satisfied only when the β_j are specifically chosen. By construction, we require that $s = \sum_{j=0}^{m-1} \beta_j$. If we choose $\beta_j = (\ln 2)^j / j!$ then

$$s = \sum_{j=0}^{m-1} \frac{(\ln 2)^j}{j!} \quad (C8)$$

becomes a truncated Taylor expansion of 2, i.e., $2 = e^{\ln 2}$. In fact, it can be shown that the required truncation order m such that $|s - 2| = \mathcal{O}(\delta)$ scales like $\log(1/\delta) / \log[\log(1/\delta)]$. With this m , it also guarantees that $\|U - \tilde{U}\| = \mathcal{O}(\delta)$, because

$$\|U - \tilde{U}\| = \left\| \sum_{j=m}^{\infty} \frac{(\ln 2)^j}{j!} V_j \right\| \leq \sum_{j=m}^{\infty} \frac{(\ln 2)^j}{j!} = |2 - s|. \quad (C9)$$

In summary, performing A on an extended system $|0\rangle |\psi\rangle$, with $\beta_j = (\ln 2)^j / j!$ and $m = \mathcal{O}[\log(1/\delta) / \log \log(1/\delta)]$, effectively performs U on $|\psi\rangle$ with $\mathcal{O}(\delta)$ accuracy.

APPENDIX D: AN ALTERNATIVE APPROACH FOR THE LCU SETUP

We provide an alternative procedure for the LCU routine that leads to an exponential saving for the state preparation. Let us define

$$\Gamma \equiv \max_{\forall k,i} \|D_i^{(k)}\|_{\max}. \quad (D1)$$

Reevaluating the coefficients in Eq. (31) using the Γ above, we have

$$\begin{aligned} & |e^{t_w x_1} e^{\Delta t_w [x_1, x_2, \dots, x_q, 0]} d_{i_q, z}^{(\mathbf{k}_q)}| \\ &= \frac{(\Gamma \tilde{\Delta} t_w e^{t_w \lambda})^q}{q!} \cos[\phi_{i_q, z}^{(\mathbf{k}_q)}] e^{i\theta_{i_q, z}^{(\mathbf{k}_q)}}. \end{aligned} \quad (D2)$$

The evolution operator from t_w to $t_w + \Delta t_w$ becomes

$$\begin{aligned} & U_I(t_w + \Delta t_w, t_w) \\ &= \sum_z U_I(t_w + \Delta t_w, t_w) |z\rangle \langle z| \\ &= \sum_z \sum_{q=0}^{\infty} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} (-i)^q \frac{(\Gamma \tilde{\Delta} t_w e^{t_w \lambda})^q}{2q!} \\ &\quad \times (e^{i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}} + e^{-i\phi_{i_q, z}^{(\mathbf{k}_q)} + i\theta_{i_q, z}^{(\mathbf{k}_q)}}) P_{\mathbf{i}_q} |z\rangle \langle z| \\ &= \sum_{q=0}^{\infty} \frac{(\Gamma \tilde{\Delta} t_w e^{t_w \lambda})^q}{2q!} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sum_{x=\pm} (-i)^q P_{\mathbf{i}_q} \Phi_{\mathbf{i}_q, x}^{(\mathbf{k}_q, w)}. \end{aligned} \quad (D3)$$

The required state $|\psi_0\rangle$ for LCU becomes

$$|\psi_0\rangle = \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{\frac{(\Gamma \widetilde{\Delta t_w} e^{t_w \lambda})^q}{2q!}} \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sum_{x=0,1} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle |x\rangle, \quad (\text{D4})$$

where s is the normalization factor, i.e.,

$$s = \sum_{q=0}^Q \frac{(MK \Gamma \widetilde{\Delta t_w} e^{t_w \lambda})^q}{q!}. \quad (\text{D5})$$

To prepare state (D4), we first prepare a state of the following form:

$$\frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{\frac{(MK \Gamma \widetilde{\Delta t_w} e^{t_w \lambda})^q}{q!}} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)} |1\rangle^{\otimes q} |0\rangle^{\otimes (Q-q)}. \quad (\text{D6})$$

Subsequently, for each $|1\rangle$ in the first Q registers ($\mathbf{i}_q$ part), we transform it to $(1/\sqrt{M}) \sum_{i=0}^M |i\rangle$, and for each $|1\rangle$ in the later Q registers ($\mathbf{k}_q$ part), we transform it to $(1/\sqrt{K}) \sum_{k=1}^K |k\rangle$. State (D6) becomes

$$\begin{aligned} & \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sqrt{\frac{(MK \Gamma \widetilde{\Delta t_w} e^{t_w \lambda})^q}{q!}} \sum_{\mathbf{i}_q} \frac{1}{\sqrt{M^q}} |\mathbf{i}_q\rangle \sum_{\mathbf{k}_q} \frac{1}{\sqrt{K^q}} |\mathbf{k}_q\rangle \\ &= \frac{1}{\sqrt{s}} \sum_{q=0}^Q \sum_{\mathbf{i}_q} \sum_{\mathbf{k}_q} \sqrt{\frac{(\Gamma \widetilde{\Delta t_w} e^{t_w \lambda})^q}{q!}} |\mathbf{i}_q\rangle |\mathbf{k}_q\rangle, \end{aligned} \quad (\text{D7})$$

which is the required $|\psi_0\rangle$ in Eq. (D4), when combined with $|x\rangle$. Note that, since the transformations $|1\rangle \rightarrow (1/\sqrt{M}) \sum_{i=0}^M |i\rangle$ and $|1\rangle \rightarrow (1/\sqrt{K}) \sum_{k=1}^K |k\rangle$ are mappings to the equally distributed state, they can be done with a column of parallel Hadamard gates, which has a gate cost $\mathcal{O}[\log(MK)]$. This provides an exponential saving compared to $\mathcal{O}(MK)$ given in the main text. This saving can be apparent when MK becomes large. However, this can create an overhead in the required number of repetitions. Indeed, we have $\Gamma e^{t_w \lambda} = MK \max_{\mathbf{i}_q, \mathbf{k}_q} \|D_i^{(k)}\|_{\max} e^{t_w \lambda}$ here compared to $\Gamma(t_w) = \sum_i \sum_k \|D_i^{(k)}\|_{\max} e^{t_w \lambda(i,k)}$ in the main text, and the overall simulation cost monotonically increases with this quantity. If only a few $\|D_i^{(k)}\|_{\max} e^{t_w \lambda(i,k)}$ are much larger than the others such that $MK \max_{\mathbf{i}_q, \mathbf{k}_q} \|D_i^{(k)}\|_{\max} e^{t_w \lambda} \gg \sum_i \sum_k \|D_i^{(k)}\|_{\max} e^{t_w \lambda(i,k)}$, then the method provided in the main text is preferred. Depending on the models, one may favor one over the other.

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