Linear combination of Hamiltonian simulation for non-unitary dynamics with optimal state preparation cost[a]

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Introduction: Fault-tolerant quantum computers are expected to perform certain unitary operations much faster than classical computers, such as simulating dynamics of a quantum state under a Hamiltonian (also known as the Hamiltonian simulation problem). However, most applications in scientific and engineering computations involve non-unitary dynamics and processes, which can often be expressed as linear differential equations of the following form

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = -A(t)u(t) + b(t), \quad u(0) = u_0. \tag{1}$$

Here $A(t) \in \mathbb{C}^{N\times N}$ is the coefficient matrix, and $b(t) \in \mathbb{C}^N$ is the inhomogeneous term [1]. Unless $A(t)$ is anti-Hermitian and $b(t) = 0$, the evolution operator of Eq. (1) denoted by $\mathcal{T}e^{-\int_0^t A(s)\,\mathrm{d}s}$ is in general non-unitary. Efficient quantum algorithms for non-unitary dynamics are the key for unlocking the full potential of quantum computers to achieve comparable speedup in these general tasks.

Contribution: In this work, we establish a surprising identity which can express *any* non-unitary dynamics as a linear combination of Hamiltonian simulation (LCHS) problems. This enables us to develop a simple quantum algorithm for simulating *general* non-unitary dynamics. We prove that LCHS can achieve optimal state preparation cost, which is useful when the initial state is difficult to prepare. Furthermore, we showcase an application in open quantum dynamics simulation using the complex absorbing potential method, which achieves near-optimal dependency on *all* parameters.

Main result: Our work establishes the following relation between non-unitary and unitary dynamics.

Theorem 1 (LCHS)**.** *Let $A(t)$ be decomposed into a Hermitian and an anti-Hermitian part as $A(t) = L(t) + iH(t)$, where $L(t) = \frac{A(t)+A^\dagger(t)}{2}$ and $H(t) = \frac{A(t)-A^\dagger(t)}{2i}$ are both Hermitian matrices. When $L(t) \succeq 0$, we have*

$$\mathcal{T}e^{-\int_0^t A(s)\,\mathrm{d}s} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T}e^{-i\int_0^t (H(s)+kL(s))\,\mathrm{d}s}\,\mathrm{d}k. \tag{2}$$

Notice that $\mathcal{T}e^{-i\int_0^t (H(s)+kL(s))\,\mathrm{d}s}$ is the unitary operator of the Hamiltonian simulation problem with a k-dependent Hamiltonian $H(s) + kL(s)$. Theorem 1 can be viewed as a generalization of the Fourier representation of the exponential function: the Fourier transform of $e^{-|x|}$ is exactly $\frac{1}{\pi(1+k^2)}$, so if $H(t) = 0$ and $L(t) = L$ is time-independent, Theorem 1 can be readily proved from the Fourier transform and the spectral mapping theorem. This special-case formula has been applied to simulating imaginary time evolution dynamics [2, 3]. However, our Theorem 1 works in a more general setting where the matrix can be time-dependent and non-Hermitian. Our general proof hinges on a special instance of the matrix version of the Cauchy integral theorem, which is a key for avoiding the spectral mapping argument.

Algorithms: By discretizing the integral with respect to k using numerical quadrature, Eq. (2) becomes $\mathcal{T}e^{-\int_0^t A(s)\,\mathrm{d}s} \approx \sum_j c_j U_{k_j}(t)$. Here c_j's are the weights, and $U_{k_j}(t)$'s are unitary operators $\mathcal{T}e^{-i\int_0^t (H(s)+k_j L(s))\,\mathrm{d}s}$. The discretized formula can be implemented either coherently on quantum computers, or in a hybrid quantum-classical fashion, as summarized in Fig. 1.

For the coherent quantum algorithm, each Hamiltonian simulation operator $U_{k_j}(t)$ can be implemented by any Hamiltonian simulation algorithm, such as high-order Trotter formula [4] and truncated Dyson series

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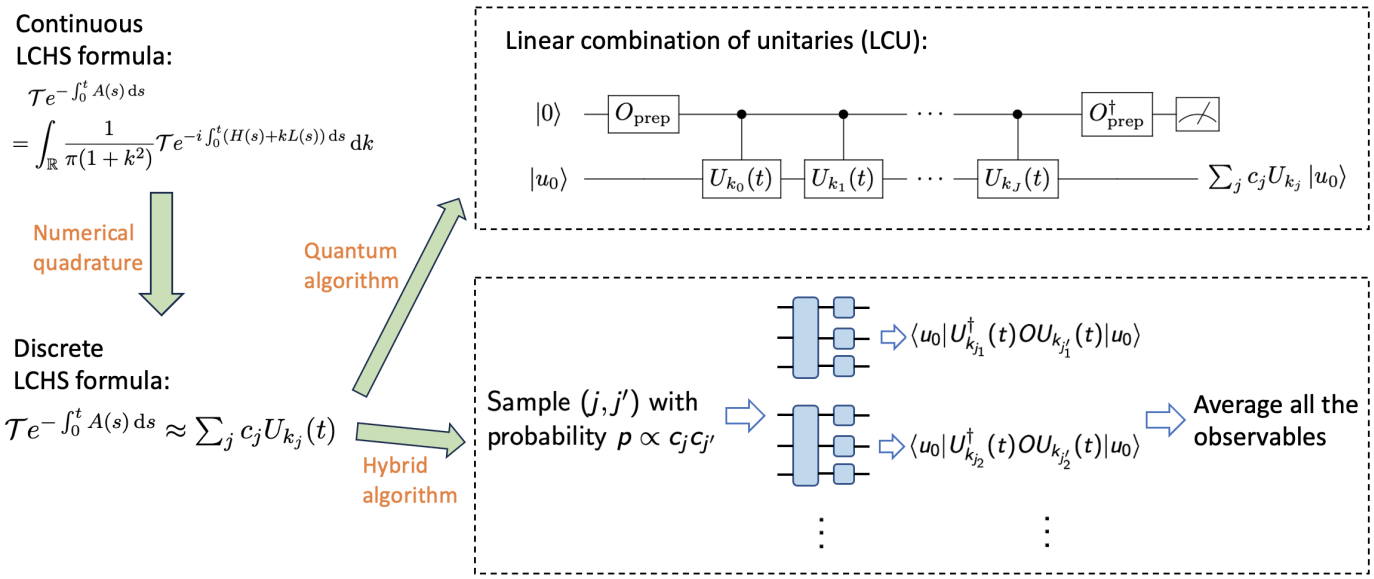


FIG. 1. Coherent implementation and hybrid quantum-classical implementation of the LCHS method.

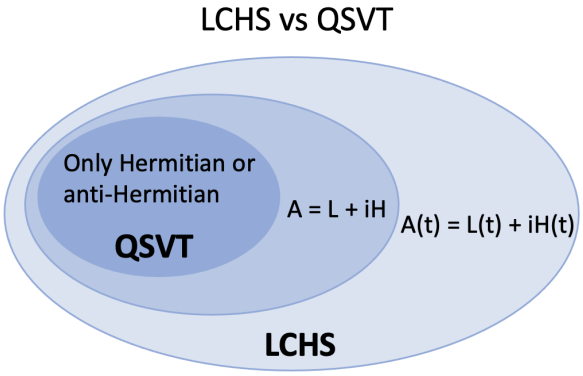
method [5]. Then the summation formula $\sum_j c_j U_{k_j}(t)$ can be efficiently implemented by the linear combination of unitaries (LCU) technique [6, 7].

If we are interested in obtaining observables of the form $u(t)^\dagger O u(t)$, it can be represented as $u(t)^\dagger O u(t) \approx \sum_{j,j'} c_j c_{j'} \langle u_0|U_{k_j}^\dagger(t) O U_{k_j'}(t)|u_0\rangle$ and can be evaluated by Monte Carlo sampling [8–10]. In particular, we first sample the index (j, j') with probability proportional to $c_j c_{j'}$, then use the quantum computer to evaluate a series of correlation functions $\langle u_0|U_{k_j}^\dagger(t) O U_{k_j'}(t)|u_0\rangle$ via the Hadamard test for non-unitary matrices [11] and amplitude estimation [12], and finally compute the average of all the sampling observables.

Comparison and complexity analysis: Recent years have witnessed significant progress in the development of efficient quantum algorithms for simulating time-independent Hamiltonians [5, 13–26] as well as time-dependent ones [4, 5, 16, 27–29]. Parallel to these advancements, substantial efforts have been made in addressing general linear differential equations [30–36]. It is noteworthy that the mechanism of LCHS stands distinct from the methodologies of these existing approaches.

We first compare LCHS with transformation-based algorithms that take advantage of the spectral mapping theorem to implement or block encode the operator $\mathcal{T}e^{-\int_0^t A(s)\,\mathrm{d}s}$. Among all the existing methods, the most general formulation is given by the quantum singular value transformation (QSVT) technique [36], which can implement a matrix function $f(A)$ where the transformation is defined over the singular values of A. When $A(t) \equiv A$, the evolution operator of ODE Eq. (1) should be implemented as an *eigenvalue transformation* of A. In the special case when A is Hermitian or anti-Hermitian, the eigenvalue transformation e^{-At} can be implemented using the *singular value transformation*. However, once A contains both Hermitian and anti-Hermitian parts or $A(t)$ becomes time-dependent, this relation no longer holds. Meanwhile, our LCHS method does not rely on the spectral mapping theorem, and is applicable to general time-dependent coefficient matrix $A(t)$ (See Fig. 2, left).

Next, we compare LCHS with other generic quantum differential equation algorithms [30–34], which convert the ODE Eq. (1) into a quantum linear system problem (QLSP). The efficiency of these quantum algorithms relies on the efficiency of the quantum linear system algorithms (QLSAs), which typically take a large number of queries to the state preparation oracle even for the state-of-the-art QLSA, as it requires multiple time evolution operators for the projector associated with the right-hand-side state of QLSP. However, our algorithm directly implements the time evolution operator by LCHS without using QLSA, and the number of the state preparation oracle is significantly reduced, as only one copy of the input state is needed in a single run of Hamiltonian simulation algorithm.



LCHS vs Dyson series

Method	Query complexity	
	A	u_0
Dyson	$\widetilde{\mathcal{O}}\left(\widetilde{q}\alpha T \log^2\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}\left(\widetilde{q}\alpha T \log\left(\frac{1}{\epsilon}\right)\right)$
LCHS	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$

FIG. 2. Comparison between LCHS and existing methods. Left: applicable ranges of LCHS and QSVT. Right: complexities in querying matrix $A(t)$ and u_0 of LCHS and truncated Dyson series method, here $\alpha = \max_t \|A(t)\|$, T is the evolution time, ϵ is the error, $q = \|u_0\|/\|u(T)\|$, and $\widetilde{q} = \max_t \|u(t)\|/\|u(T)\|$ (we always have $q \le \widetilde{q}$).

In Fig. 2 (right), we compare the query complexity of our LCHS method with the best existing quantum differential equation algorithm, which combines the truncated Dyson series with QLSA [34]. The LCHS method only needs $\mathcal{O}(\|u_0\|/\|u(T)\|)$ queries to the state preparation oracle of $|u_0\rangle$, which is much better than that of the truncated Dyson series method because the truncated Dyson series method uses QLSA as its subroutine. In fact, the $\mathcal{O}(\|u_0\|/\|u(T)\|)$ scaling is optimal and matches the lower bound [37]. The drawback of the LCHS method is the $\mathcal{O}(1/\epsilon)$ dependence in the number of queries to $A(t)$. This is because we need to simulate the Hamiltonian $H(s)+kL(s)$ for very large $k \sim 1/\epsilon$ due to the slow decay of the kernel $\frac{1}{\pi(1+k^2)}$. We remark that such a scaling can be significantly improved for certain applications, including simulating certain open quantum dynamics problems (see below).

Application: We apply our LCHS method to simulating open quantum system dynamics with complex absorbing potentials [38–40], which has many applications such as molecular scattering and photodissociation:

$$i\frac{\mathrm{d}}{\mathrm{d}t}u(t) = \left(-\frac{1}{2}\Delta_{\mathbf{r}} + V_R(t) - iV_I\right)u(t). \tag{3}$$

Here $V_R(t)$ is the time-dependent external potential, and V_I is the absorbing potential, which is a local potential in the real space that satisfies $V_I(\mathbf{r}) \ge 0$. Therefore, we may directly let $L = V_I$ and $H(t) = -\frac{1}{2}\Delta + V_R(t)$ and apply the LCHS method.

Notice that in this application, the Hermitian part $L = V_I$ is time-independent and fast-forwardable, in the sense that e^{-ikLt} can be performed with cost independent of k, t and $\|L\|$ [41]. We may take advantage of this feature to further speed up the implementation of LCHS. Instead of directly simulating $H(t) + kL$ which has large spectral norm for large k, we may simulate the dynamics in the interaction picture [5] by propagating the quantum state rotated by e^{ikLt}. The resulting Hamiltonian becomes $H_I(s;k) = e^{iLks}H(s)e^{-iLks}$, which is bounded and can be efficiently simulated using truncated Dyson series method [5]. The overall complexity is almost independent of k (depends at most poly-logarithmically on k). Therefore, by combining LCHS with Hamiltonian simulation in the interaction picture, we avoid the computational overhead brought by the large truncation order of k and further reduce the number of queries to the matrix oracles.

We summarize the complexity of LCHS in simulating open quantum dynamics with complex absorbing potentials as follows. Remarkably, it achieves **near-optimal scaling in all parameters**. We also note that the following result also holds in a more general case where $H(t)$ is an arbitrary time-dependent Hamiltonian and L is a time-independent fast-forwardable Hamiltonian.

Theorem 2. *Consider simulating open quantum dynamics with complex absorbing potentials in Eq. (3). Then the LCHS method with interaction picture Hamiltonian simulation can prepare an ϵ-approximation of the state*

$|u(T)\rangle$ with $\Omega(1)$ success probability and a flag indicating success, using

$$\widetilde{\mathcal{O}}\left(\frac{\|u_0\|}{\|u(T)\|}T(\max_t \|H(t)\|)\ \mathrm{polylog}\left(\frac{1}{\epsilon}\right)\right) \tag{4}$$

queries to the matrix input oracles, and $\mathcal{O}(\|u_0\|/\|u(T)\|)$ queries to the state preparation oracle of $|u_0\rangle$.

[1] In this extended abstract we mainly focus on the homogeneous case where $b(t) \equiv 0$, but all the results can be easily generalized to the inhomogeneous case (also discussed in the paper).
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