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Linear Combination of Hamiltonian Simulation for Nonunitary Dynamics with Optimal State Preparation Cost

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We propose a simple method for simulating a general class of nonunitary dynamics as a linear combination of Hamiltonian simulation (LCHS) problems. LCHS does *not* rely on converting the problem into a dilated linear system problem or on the spectral mapping theorem. The latter is the mathematical foundation of many quantum algorithms for solving a wide variety of tasks involving nonunitary processes, such as the quantum singular value transformation. The LCHS method can achieve optimal cost in terms of state preparation. We also demonstrate an application for open quantum dynamics simulation using the complex absorbing potential method with near-optimal dependence on all parameters.

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Introduction.—Fault-tolerant quantum computers are expected to excel in simulating unitary dynamics, such as the dynamics of a quantum state under a Hamiltonian. Most applications in scientific and engineering computations involve nonunitary dynamics and processes. Therefore, efficient quantum algorithms are the key for unlocking the full potential of quantum computers to achieve comparable speedup in these general tasks. Quantum phase estimation (QPE) [1,2] is the first algorithm to bridge this gap. QPE stores the eigenvalues of the Hamiltonian in an ancilla quantum register, and can be used to solve a wide range of problems, including amplitude estimation [3], linear systems [4], and differential equations [5,6]. There have been two significant improvements over QPE-based methods. The first is linear combination of unitaries (LCU) [7], which provides an exponential improvement in precision for tasks such as the Hamiltonian simulations [8,9] and linear systems [10]. Here the exponential improvement refers to the cost of preparing a quantum state in a register, which also directly translates into a polynomial improvement in precision when the final measurement cost is taken into account. The second is quantum signal processing (QSP) [11] and its generalization, including quantum singular value transformation (QSVT) [12] and quantum eigenvalue transformation of unitary matrices [13]. Compared to LCU, QSP-based approaches can achieve a similar level of accuracy but with a much more compact quantum circuit and a minimal number of ancilla qubits.

The unifying mathematical argument that underlies many of these approaches is the spectral mapping theorem for Hermitian matrices: Let A be a Hermitian matrix and $f(A)$ be a real-valued matrix function defined on the eigenvalues of A. Then, the eigenvalues of the matrix $f(A)$ are equal to the values of the classical function f applied to the eigenvalues of A, i.e., if $\lambda_1, \ldots, \lambda_N$ are the eigenvalues of A, then the eigenvalues of $f(A)$ are $f(\lambda_1), \ldots, f(\lambda_N)$. Furthermore, $f(A)$ is diagonalized by the same unitary matrix that diagonalizes A. For instance, the quantum linear system problem corresponds to $f(A) = A^{-1}$, Hamiltonian simulation corresponds to $f(A) = \cos(At), \sin(At)$ (for the real and imaginary parts of e^{-iAt}), and Gibbs state preparation corresponds to $f(A) = e^{-A}$.

The limitation of this matrix-function-based perspective can be readily observed when solving a general differential equation,

$$\partial_t u(t) = -A(t)u(t) + b(t), \qquad u(0) = u_0. \tag{1}$$

When $b(t) = 0$ and $A(t) = A \in \mathbb{C}^{N\times N}$ is a general time-independent matrix, the system has a closed form solution $u(t) = e^{-At}u_0$. Even in this case, the eigenvalues of A may not be real, the eigenvectors of A may not form a unitary matrix, or A may not be diagonalizable at all. These

difficulties prevent us from applying techniques such as QSVT to implement $f(A) = e^{-At}$ on a quantum computer, and the situation becomes much more complicated when A, b are not some fixed matrices and vectors, but are time dependent. To solve Eq. (1), most existing quantum algorithms convert the problem into a quantum linear system problem (QLSP) with a fixed and dilated matrix (i.e., a matrix of enlarged size). The resulting QLSP can then be solved using many of the aforementioned techniques based on the spectral mapping argument. However, both the construction of the linear system problem and the solution of the QLSP with near-optimal complexity (in order to achieve desired dependence on parameters such as the precision and the simulation time) can be very involved. We shall compare our new proposals with the QLSP approach later in the Letter.

In this Letter, we propose a significantly simplified solution to the nonunitary process in Eq. (1). Our procedure is not based on the spectral mapping theorem, but on a surprising identity expressing the solution as a linear combination of Hamiltonian simulation (LCHS) problems. LCHS can be viewed as a special case of LCU. Namely, each Hamiltonian simulation problem is described by a unitary operator. Unlike LCU for Hamiltonian simulation or solving linear systems, these unitary operators do not commute with each other. LCHS is a very flexible procedure. The linear combination can be implemented in a hybrid quantum-classical fashion to compute observables related to the solution, using a small amount of quantum resources, and is thus suitable for the setting of early fault-tolerant quantum computers. The linear combination can also be coherently implemented to prepare the solution directly in a quantum register and to reduce the complexity. In this case, we show that the cost of LCHS is optimal in terms of state preparation, which is useful when the initial state u_0 is difficult to prepare.

When the anti-Hermitian part of the matrix $A(t)$ is fast-forwardable, we may incorporate the interaction picture Hamiltonian simulation in the LCHS to obtain further improvements. A practical example with such a feature is the open quantum system dynamics. Many problems in quantum dynamics, such as molecular scattering [14], photodissociation [15], and nanotransport [16], are defined in an infinite space. Unlike solving the ground state of molecules in quantum chemistry, replacing the infinite space by a finite-sized box in these quantum dynamics problems may lead to significant errors, at least along certain extended dimensions. Therefore, boundary conditions need to be carefully designed and implemented to balance the accuracy of the simulation and the computational cost. One widely used method in quantum chemistry is the complex absorbing potential (also called the imaginary potential) method [15,17,18]. In this case, we show that our LCHS algorithm can achieve near-optimal dependence on *all* parameters in both state preparation and matrix input models.

Linear combination of Hamiltonian simulation.—Let us consider the homogeneous problem first with $b(t) = 0$.

Theorem 1.—Let $A(t) \in \mathbb{C}^{N\times N}$, $t \in \mathcal{I} = [0, T]$ be decomposed into a Hermitian and an anti-Hermitian part, $A(t) = L(t) + iH(t)$, where $L(t) = [A(t) + A^\dagger(t)]/2$ and $H(t) = [A(t) - A^\dagger(t)]/2i$. Assume $L(t) \geq 0$ for all $t \in \mathcal{I}$. Then ($\mathcal{T}$ is the time ordering operator),

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

Theorem 1 can be viewed as a generalization of the Fourier representation of the exponential function $f(x) = e^{-|x|}$,

$$\hat{f}(k) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{-|x|} e^{-ikx} dx = \frac{1}{\pi(1+k^2)}. \tag{3}$$

Note that $\hat{f}(k) \geq 0$ and $\int \hat{f}(k)dk = 1$. Therefore, $\hat{f}(k)$ is the density of a probability distribution, called the Cauchy-Lorentz distribution. If $H(t) = 0$ and $L(t) = L$ is time independent, Theorem 1 can be readily proved from Eq. (3) and the spectral mapping theorem. This special-case formula has been applied to simulating imaginary time evolution dynamics [19,20]. 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 (see the Supplemental Material [21]).

The condition that the Hermitian part $L(t)$ is positive semidefinite can always be satisfied without loss of generality. Indeed, by redefining $u(t) = e^{ct}v(t)$, the equation for $v(t)$ is

$$\partial_t v(t) = -[L(t) + cI + iH(t)]v(t) + e^{-ct}b(t), \quad v(0) = u_0. \tag{4}$$

By choosing $-c$ to be the minimum of the smallest eigenvalues of $L(t)$ on $t \in \mathcal{I}$, $L(t) + cI$ is a positive semidefinite matrix.

When $b(t) = 0$, the solution to Eq. (1) becomes $u(t) = \mathcal{T} e^{-\int_0^t A(s)ds} u_0$. By discretizing the integral with respect to k using a grid k_j with quadrature weights ω_j, Eq. (2) becomes

$$u(t) \approx \sum_j c_j U_j(t) u_0, \tag{5}$$

where $c_j = \omega_j/\pi(1+k_j^2)$, and $U_j(t) = \mathcal{T} e^{-i\int_0^t [H(s)+k_jL(s)]ds}$ is the propagator for a time-dependent Hamiltonian simulation problem. Therefore, Eq. (2) compactly expresses the

solution as a problem of LCHS, which can be coherently implemented using LCU (see the Supplemental Material [21]).

If we are only interested in obtaining observables of the form $u(t)^* O u(t)$, we may implement the linear combination in a hybrid quantum-classical fashion. Notice that, since U_j's are unitary, the observable can be expressed as

$$u(t)^* O u(t) \approx \sum_{k,k'} c_k^* c_{k'} \langle u_0 | U_k^\dagger(t) O U_{k'}(t) | u_0 \rangle. \quad (6)$$

We can then use the quantum computer to evaluate a series of correlation functions $\langle u_0 | U_k^\dagger(t) O U_{k'}(t) | u_0 \rangle$ via the Hadamard test for nonunitary matrices [22] and amplitude estimation [3], and perform the summation on a classical computer [23–25] (see the Supplemental Material [21]).

In the presence of the source term $b(t)$, we can use the Duhamel's principle (also known as variation of constants) to express the solution as

$$u(t) = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T} e^{-i\int_0^t [H(s)+kL(s)]ds} u_0 dk + \int_0^t \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T} e^{-i\int_s^t [H(s')+kL(s')]ds'} b(s) dk ds. \quad (7)$$

We may again use LCU to coherently prepare the state $u(t)$ or use an expression similar to that of Eq. (6) for hybrid computation of observables.

Implementation.—The LCHS can be implemented in a gate-efficient way by combining LCU with any Hamiltonian simulation algorithms. Here we discuss the simplest implementation of LCHS based on the product formula, and we will discuss the one based on the truncated Dyson series method later in the Letter.

We first truncate the integral in Eq. (2) on a finite interval $[-K, K]$ and discretize it by a trapezoidal rule with $(M+1)$ grid points. We obtain $\mathcal{T} e^{-\int_0^t A(s)ds} u_0 \approx \sum_{j=0}^M c_j \mathcal{T} e^{-i\int_0^t [H(s)+k_j L(s)]ds} u_0$. Here $c_j = w_j/\pi(1+k_j^2)$, $w_j = (2 - \mathbf{1}_{j=0,M})K/M$, and $k_j = -K + 2jK/M$ are the weights and nodes of the trapezoidal rule. To implement each $U_j(t) = \mathcal{T} e^{-i\int_0^t [H(s)+k_j L(s)]ds}$, we use a pth order product formula with a fixed number of steps r for all j. Then,

$$\mathcal{T} e^{-\int_0^t A(s)ds} u_0 \approx \sum_{j=0}^M c_j v_j, \quad v_j = \prod_{l'=0}^{r-1} \prod_{l=0}^{\Xi_p - 1} \left(e^{-iH\left(\frac{(l'+\delta_l)t}{r}\right)\frac{\beta_l t}{r}} e^{-iL\left(\frac{(l'+\gamma_l)t}{r}\right)\frac{\alpha_l k_j t}{r}} \right) u_0. \quad (8)$$

Here Ξ_p is the number of the exponentials in the product formula, α_l's and β_l's are the corresponding coefficients, and γ_l's and δ_l's determine the discrete times at which the time-dependent Hamiltonians are evaluated (see Ref. [26] for an example of the product formula via Suzuki recursion).

Suppose that we are given the state preparation oracle $O_{\text{prep}}\colon |0\rangle \to |u_0\rangle$, the Hamiltonian simulation oracles $O_L(s,\tau) = e^{-iL(\tau)s}$ for $|s| \le 1/\|L\|$ and $O_H(s,\tau) = e^{-iH(\tau)s}$ for $|s| \le 1/\|H\|$, and the LCU coefficient oracle $O_{\text{coef}}\colon |0\rangle \to (1/\sqrt{\|c\|_1}) \sum_{j=0}^M \sqrt{c_j} |j\rangle$. According to the binary representations of j's, we may first construct a coherent encoding of the time evolution as the select oracle $\text{SEL}_L(s,\tau) = \sum_{j=0}^M |j\rangle\langle j| \otimes e^{-iL(\tau)k_j s}$ using $\mathcal{O}[\log(M)]$ queries to $O_L(s,\tau)$ (see Supplemental Material [21] and, e.g., [10,27,28] for details). Then Eq. (8) can be implemented following the standard LCU approach by first applying $O_{\text{coef}} \otimes O_{\text{prep}}$, then sequentially applying $\text{SEL}_L(\alpha_l t/r, (l'+\gamma_l)t/r)$ and $O_H(\beta_l t/r, (l'+\delta_l)t/r)$ for $l \in [\Xi_p]$ and $l' \in [r]$, and finally applying $O_{\text{coef}}^\dagger$ on the ancilla register. Such a procedure yields the quantum state approximating $(1/\|c\|_1 \|u_0\|)|0\rangle_a \mathcal{T} e^{-\int_0^t A(s)ds} u_0 + |\perp\rangle$, encoding the homogeneous part in its first subspace.

For the inhomogeneous term in Eq. (7), after discretizing the integral for both k and s using the multidimensional trapezoidal rule, we obtain $\int_0^t \mathcal{T} e^{-\int_s^t A(s')ds'} b(s) ds \approx \sum_{j'=0}^{M_t} \sum_{j=0}^M \tilde{c}_{j,j'} \mathcal{T} e^{-i\int_{s_{j'}}^t [H(s')+k_j L(s')]ds'} |b(s_{j'})\rangle$. Here $\tilde{c}_{j,j'} = v_{j'} w_j \|b(s_{j'})\|/\pi(1+k_j^2)$, w_j, k_j are as defined before, $v_{j'} = (2 - \mathbf{1}_{j'=0,M})T/2M_t$, and $s_{j'} = j'T/M_t$. This can also be implemented by the same Trotterization and LCU approach as the homogeneous case (see Supplemental Material for details [21]). Notice that the evolution time of different Hamiltonians in the LCHS of the inhomogeneous term varies, so we will assume the input model of H, L to coherently encode the evolution of different Hamiltonians with different time periods, as $O'_L(s,\tau_0,\tau_1) = \sum_{j'=0}^{M_t} |j'\rangle\langle j'| \otimes e^{-iL[\tau_0 j' + \tau_1(M_t - j')]s(M_t - j')}$ and $O'_H(s,\tau_0,\tau_1) = \sum_{j'=0}^{M_t} |j'\rangle\langle j'| \otimes e^{-iH[\tau_0 j' + \tau_1(M_t - j')]s(M_t - j')}$ for $|s| M_t \le 1/\|H\|$. The input for $b(t)$ is also in a time-dependent manner as $O_b\colon |j'\rangle|0\rangle \to |j'\rangle|b(s_{j'})\rangle$. All of these oracles are an extension of the time-dependent encoding proposed in [27].

To linearly combine $\mathcal{T} e^{-\int_0^t A(s)ds} u_0$ and $\int_0^t \mathcal{T} e^{-\int_s^t A(s')ds'} b(s) ds$, we append an extra ancilla qubit, prepare both states controlled by this ancilla qubit, and implement the LCU again at the outer loop using a single-qubit rotation. The final step is to measure all the ancilla registers, and if all the outcomes are zero, then the resulting state approximately encodes the solution $u(t)$ of the ordinary differential equation.

Computational cost.—The complexity of our algorithm for solving Eq. (1) is given as follows. Here $|u(T)\rangle$ is the solution to Eq. (1) at the final time T.

Theorem 2.—There exists a quantum algorithm that prepares an ϵ approximation of the state $|u(T)\rangle$ with $\Omega(1)$ success probability and a flag indicating success, using

(1) queries to the aforementioned input models of H and L a total number of times

$$\tilde{\mathcal{O}}\left(\left(\frac{\|u_0\|+\|b\|_{L^1}}{\|u(T)\|}\right)^{2+2/p}\frac{\Gamma_p^{1+1/p}T^{1+1/p}}{\epsilon^{1+2/p}}\right), \tag{9}$$

where $\|b\|_{L_1}=\int_0^T\|b(s)\|ds$ and $\Gamma_p=\max_{0\le q\le p,\tau\in[0,T]}(\|H^{(q)}(\tau)\|+\|L^{(q)}(\tau)\|)^{1/(q+1)}$,

(2) queries to the state preparation oracle O_{prep} and the source term input model O_b for $\mathcal{O}\left((\|u_0\|+\|b\|_{L^1})/\|u(T)\|\right)$ times,

(3) $\mathcal{O}[\log(\Gamma_1\|b\|_{C^2}T/\epsilon)]$ ancilla qubits, where $\|b\|_{C^2}=\max_{0\le q\le 2,\tau\in[0,T]}(\|b^{(q)}(\tau)\|)$,

(4) $\mathcal{O}\left((\|u_0\|+\|b\|_{L^1})/\|u(T)\|\right)$ additional 1-qubit gates.

The proof of Theorem 2 can be found in the Supplemental Material [21]. Our algorithm uses a small number of queries to the state preparation oracle. This is because each run of the LCU procedure only requires $\mathcal{O}(1)$ uses of such oracles and the overall complexity only relates to the success probability, which contributes to a $(\|u_0\|+\|b\|_{L^1})/\|u(T)\|$ factor. The query complexity to the matrix input in each run depends linearly on the number of time steps, which contributes to the scaling $\Gamma_p^{1+1/p}T^{1+1/p}/\epsilon^{1/p}$ according to the pth order product formula error bound. The extra $1/\epsilon^{1/p}$ scaling is due to the relative error scaling. Notice that in the matrix query complexity there are still extra terms including $1/\epsilon$ and $[(\|u_0\|+\|b\|_{L^1})/\|u(T)\|]^{1+1/p}$. The former is because we need to simulate the Hamiltonian up to $K=\mathcal{O}(\epsilon^{-1})$, while the latter arises from the necessity of bounding the relative Trotter error. Ancilla qubits are used to implement quadrature.

Our algorithm and Theorem 2 can be directly applied to the special case where $A(t)\equiv A$ is time independent. In this case, we may further simplify the implementation and reduce the computational cost. First, the coherent encoding of the time evolution is no longer needed, and the select oracles in the LCU procedure can be efficiently constructed using $O_L(s)=e^{-iLs}$ and $O_H(s)=e^{-iHs}$ with $\mathcal{O}[\log(M)\log(M_t)]$ cost. Second, the parameter Γ_p can be improved to the commutator scalings between H and L thanks to the improved error bound for time-independent product formula [29]. We refer the reader to the Supplemental Material for more details [21].

Optimal state preparation cost and comparison with other methods.—The query complexity of the LCHS approach to the state preparation oracle O_{prep} is $\mathcal{O}\left[(\|u_0\|+\|b\|_{L^1})/\|u(T)\|\right]$. In fact, when $b=0$, this corresponds to the dependence of a quantity denoted by $q=\|u_0\|/\|u(T)\|$ in quantum differential equation solvers. Such a linear scaling of q cannot be improved. From the perspective of quantum complexity theory, the renormalization from $\|u_0\|$ to $\|u(T)\|$ could be utilized to implement postselection, and it would imply the unlikely consequence BQP = PP (similar discussions appear in Sec. 8 of [30] and Sec. 7 of [31]). Moreover, as shown in Corollary 16 of [32], any quantum differential equation algorithm must have worst-case query complexity $\Omega(q)$ to the state preparation oracle, indicating the optimal state preparation cost that our LCHS approach achieves.

Most generic quantum differential equation algorithms [5,6,30,33,34] convert the time-dependent differential equation problem (1) into a QLSP. The efficiency of these quantum algorithms relies on the efficiency of the quantum linear system algorithm (QLSA), which typically takes a large number of queries to the state preparation oracle. In particular, the state-of-the-art QLSA takes $\mathcal{O}[\kappa\log(1/\epsilon)]$ queries [35], where κ is the condition number of the QLSP matrix and depends on T and $\|A(t)\|$. However, our algorithm directly implements the time evolution operator by LCHS without using the QLSA, so the number of the state preparation oracle is significantly reduced. For example, when $b=0$, our algorithm takes $\mathcal{O}\left(\|u_0\|/\|u(T)\|\right)$ queries to the state preparation, while the state-of-the-art QLSA-based quantum Dyson series method [34] queries the initial state $\mathcal{O}\left\{[\|u_0\|/\|u(T)\|]\|A\|T\log(1/\epsilon)\right\}$ times. Our algorithm removes the explicit dependence on $\|A\|$, T, and ϵ and matches the lower bound. Additionally, in the QLSA-based approaches, the value of κ can be difficult to estimate in practice, and it is common that the theoretical bound significantly overestimates the value of κ [33]. We also note that the time marching method [36] does not involve QLSP and can query the initial state $\mathcal{O}\left(\|u_0\|/\|u(T)\|\right)$ times as well. In this case, our LCHS approach removes the need of implementing the uniform singular value amplification procedure and can thus be simpler to implement. It also outperforms the time marching method in terms of the number of matrix queries with respect to the evolution time, with an improvement from $\mathcal{O}(T^2)$ to $\mathcal{O}(T^{1+o(1)})$.

Applications to open quantum system dynamics with complex absorbing potentials.—In its simplest form, the complex absorbing potential method [15,17,18] replaces the real potential by a complex one, and the time-dependent Schrödinger equation becomes

$$i\partial_t u(\mathbf{r},t)=\left(-\frac{1}{2}\Delta_{\mathbf{r}}+V_R(\mathbf{r},t)-iV_I(\mathbf{r})\right)u(\mathbf{r},t). \tag{10}$$

Here $V_R(\mathbf{r},t)$ is the real time-dependent external potential, and $-iV_I(\mathbf{r})$ is the absorbing potential and can often be chosen to be time independent. The minus sign reflects that this is a damping potential, and V_I can be chosen to be bounded and non-negative. For simplicity, we only discuss Eq. (10) in the context of single-particle dynamics. This formulation can be generalized to accommodate multi-particle dynamics. Our method can also be generalized to other boundary treatment methods such as the perfectly matched layer method [37,38]. In these applications, we are interested in the case before the scattering wave leaves the region of interest, i.e., $\|u(T)\|^2 = \int |u(\mathbf{r},T)|^2 d\mathbf{r}$ is not too small. Such a condition can also be satisfied if u_0 is a near-resonance state. Another widely used method for modeling open quantum system dynamics is the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) quantum master equation [39–41]. The non-Hermitian quantum dynamics (10) is also related to a class of numerical methods for solving the GKSL equation, known as the quantum jump or the Monte Carlo wave function method [42,43].

To solve Eq. (10) using our LCHS algorithm, we first discretize the spatial variable using N equidistant grid points, and the Laplace operator is discretized by the central difference formula. In the context of Eq. (1), the Hermitian part $H(t) = -\frac{1}{2}\Delta_{\mathbf{r}} + V_R(t)$ is the standard Hamiltonian with $\|H(t)\| = \mathcal{O}(N^2 + \max_t \|V_R(t)\|)$, and the non-Hermitian part $L = V_I$ is a time-independent positive semidefinite matrix. Furthermore, the dynamics e^{-ikLt} can be fast-forwarded in the sense that e^{-ikLt} can be performed with cost independent of k, t, and $\|L\|$ [44], so we may perform the Hamiltonian simulation in the interaction picture with the truncated Dyson series method [27] to avoid computational overhead brought by K.

In the interaction picture, the LCHS becomes

$$\mathcal{T} e^{-\int_0^t A(s)ds} \approx \sum_{j=0}^{M} c_j e^{-iLk_j t} \left(\mathcal{T} e^{-i\int_0^t H_I(s;k_j)ds} \right) e^{iLk_j t}, \quad (11)$$

where $H_I(s;k) = e^{iLks} H(s) e^{-iLks}$. Equation (11) can be directly implemented by LCU. Notice that the derivative of H_I still scales linearly in K, but the cost of the truncated Dyson series method scales only logarithmically with respect to the derivative of $H_I(s)$ and thus K [27].

Our main result is as follows, which achieves near-optimal scaling in *all* parameters. The proof is given in the Supplemental Material [21]. We remark 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 3.—Consider the spatially discretized Eq. (10) using finite difference with N equidistant grid points. Suppose that we are given the oracles $O_{V_I}\colon |\mathbf{r}\rangle|0\rangle \to |\mathbf{r}\rangle|V_I(\mathbf{r})\rangle$, $O_{V_R}\colon |\mathbf{r}\rangle|s\rangle|0\rangle \to |\mathbf{r}\rangle|s\rangle|V_R(\mathbf{r},s)\rangle$, and the state preparation oracle O_{prep} for the initial condition. Then there exists a quantum algorithm that prepares an ϵ approximation of the discretized state $|u(T)\rangle$ with $\Omega(1)$ success probability and a flag indicating success, using

$$\tilde{\mathcal{O}}\left[\frac{\|u_0\|}{\|u(T)\|} T(\max_t \|H(t)\|) \operatorname{poly}\log\left(\frac{\max_t \|V_R'(t)\| \|V_I\|}{\epsilon} \right) \right] \quad (12)$$

queries to O_{V_I} and O_{V_R}, and $\mathcal{O}(\|u_0\|/\|u(T)\|)$ queries to O_{prep}. Here $\max_t \|H(t)\| = \mathcal{O}(N^2 + \max_t \|V_R(t)\|)$.

Discussion.—LCHS provides a simple way for solving the nonunitary dynamics in the form of Eq. (1). Compared to existing approaches based on QLSP, LCHS is simple, flexible, and achieves optimal state preparation cost. The linear combination procedure can be implemented in a hybrid quantum-classical fashion to facilitate the computation of observables on early fault-tolerant quantum computers. The most significant limitation of LCHS is that the spectral radius of the Hermitian part L needs to be multiplied by a factor up to the frequency cutoff K, where $K = \mathcal{O}(1/\epsilon)$ due to the quadratic decay of the kernel $(1+k^2)^{-1}$. This increases the maximal circuit depth by a factor ϵ^{-1}. The problem can be ameliorated when the dynamics of L can be fast-forwarded. For instance, in the case of simulating open quantum system dynamics using a complex absorbing potential, our LCHS-based solver achieves near-optimal complexity in all parameters. However, Hamiltonian simulation in the interaction picture [27] may be difficult to implement. A more desirable solution to this problem would be to replace the kernel $(1+k^2)^{-1}$ by a fast decaying one, so that the truncation range can be dramatically reduced. It remains an open question how to obtain the best possible solver that is optimal in all parameters for simulating general nonunitary dynamics.

When a task can be solved using either LCU or QSP-based techniques, the latter are often preferred due to their superior resource efficiency, as well as ease of implementation. However, all QSP-based techniques are based on the spectral mapping theorem. LCHS avoids this spectral mapping argument and thus significantly expands the application range of LCU. It would be interesting to see if the mathematical reformulation of LCHS can inspire further generalization of QSP-based approaches, particularly for applications involving non-normal matrices. Additionally, exploring extensions of LCHS to other quantum linear algebra problems can be a promising direction for future research.

Note added.—Recently, we became aware of a recent work called "Schrödingerisation" [45], which transforms a general class of linear partial differential equations into a

dilated Hamiltonian dynamics and can be used to provide a complementary perspective of our result in Theorem 1.

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