Efficient Quantum Algorithms for Simulating Lindblad Evolution*†

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— Abstract -

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We consider the natural generalization of the Schrödinger equation to Markovian open system dynamics: the so-called the Lindblad equation. We give a quantum algorithm for simulating the evolution of an n-qubit system for time t within precision ϵ . If the Lindbladian consists of poly(n) operators that can each be expressed as a linear combination of poly(n) tensor products of Pauli operators then the gate cost of our algorithm is $O(t \operatorname{polylog}(t/\epsilon)\operatorname{poly}(n))$. We also obtain similar bounds for the cases where the Lindbladian consists of local operators, and where the Lindbladian consists of sparse operators. This is remarkable in light of evidence that we provide indicating that the above efficiency is impossible to attain by first expressing Lindblad evolution as Schrödinger evolution on a larger system and tracing out the ancillary system: the cost of such a reduction incurs an efficiency overhead of $O(t^2/\epsilon)$ even before the Hamiltonian evolution simulation begins. Instead, the approach of our algorithm is to use a novel variation of the "linear combinations of unitaries" construction that pertains to channels.

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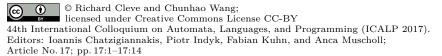
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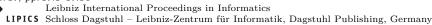
1 Introduction

The problem of simulating the evolution of closed systems (captured by the Schrödinger equation) was proposed by Feynman [12] in 1982 as a motivation for building quantum computers. Since then, several quantum algorithms have appeared for this problem (see section 1.1 for references to these algorithms). However, many quantum systems of interest are not closed but are well-captured by the Lindblad Master equation [21, 13]. Examples exist in quantum physics [20, 32], quantum chemistry [25, 27], and quantum biology [11, 14, 26]. Lindblad evolution also arises in quantum computing and quantum information in the

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Figure 1 Lindblad evolution for time t approximated by unitary operations. There are N iterations and $\delta = t/N$. This converges to Lindblad evolution as $N \to \infty$.

context of entanglement preparation [19, 16, 29], thermal state preparation [15], quantum state engineering [31], and studying the noise of quantum circuits [24].

We consider the computational cost of simulating the evolution of an n-qubit quantum state for time t under the Lindblad Master equation

$$\dot{\rho} = -i[H, \rho] + \sum_{j=1}^{m} \left(L_j \rho L_j^{\dagger} - \frac{1}{2} L_j^{\dagger} L_j \rho - \frac{1}{2} \rho L_j^{\dagger} L_j \right), \tag{1}$$

(representing Markovian open system dynamics), where H is a Hamiltonian and L_1, \ldots, L_m are linear operators. By *simulate the evolution*, we mean: provide a quantum circuit that computes the quantum channel corresponding to evolution by Eq. (1) for time t within precision ϵ . The quantum circuit must be independent of the input state, which is presumed to be unknown. When $L_1 = \cdots = L_m = 0$, Eq. (1) is the Schrödinger equation.

Eq. (1) can be viewed as an idealization of the frequently occurring physical scenario where a quantum system evolves jointly with a large external environment in a manner where information dissipates from the system into the environment. In quantum information theoretic terms, Lindblad evolution is a continuous-time process that, for any evolution time, is a quantum channel. Moreover, Lindblad evolution is Markovian in the sense that, for any $\delta > 0$, the state at time $t + \delta$ is a function of the state at time t alone (i.e., is independent of the state before time t).

Lindblad evolution can be intuitively thought of as Hamiltonian evolution in a larger system that includes an ancilla register, but where the ancilla register is being continually reset to its initial state. To make this more precise, consider a time interval [0,t], and divide it into N subintervals of length $\frac{t}{N}$ each. At the beginning of each subinterval, reset the state of the ancilla register to its initial state, and then let the joint system-ancilla evolve under a Hamiltonian J and the system itself evolve under H. Let the evolution time for J be $\sqrt{t/N}$ and the evolution time for H be t/N. This process, illustrated in Fig. 1, converges to true Lindblad evolution as N approaches ∞ .

For the specific evolution described by Eq. (1), it suffices to set the ancilla register to \mathbb{C}^{m+1} and the Hamiltonian J to the block matrix

$$J = \begin{pmatrix} 0 & L_1^{\dagger} & \cdots & L_m^{\dagger} \\ L_1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_m & 0 & \cdots & 0 \end{pmatrix}. \tag{2}$$

A remarkable property of this way of representing Lindblad evolution is that the rate at which the Hamiltonian J evolves is effectively infinite: Lindblad evolution for time t/N is simulated by a process that includes evolution by J for time $\sqrt{t/N}$, so the rate of the

evolution scales as

$$\frac{\sqrt{t/N}}{t/N} = \sqrt{\frac{N}{t}},\tag{3}$$

which diverges as $N \to \infty$. Moreover, the total Hamiltonian evolution time of J in Fig. 1 is $N\sqrt{t/N} = \sqrt{Nt}$, which also diverges. In the Appendix A we prove that, in general, the above scaling phenomenon is necessary for simulating time-independent Lindblad evolution in terms of time-independent Hamiltonian evolution along the lines of the overall structure of Fig. 1. In this sense, exact Lindblad evolution for finite time does not directly correspond to Hamiltonian evolution for any finite time. On the other hand, it can be shown that if the scaling of N is at least t^3/ϵ^2 then the final state is an approximation within ϵ . Note that then the corresponding total evolution time for J scales as $\sqrt{(t^3/\epsilon^2)t} = t^2/\epsilon$. Therefore, quantum algorithms that simulate Lindblad evolution by first applying the above reduction to Hamiltonian evolution and then efficiently simulating the Hamiltonian evolution are likely to incur scaling that is at least t^2/ϵ .

Here we are interested in whether much more efficient simulations of Lindblad evolution are possible, such as $O(t \operatorname{polylog}(t/\epsilon))$.

1.1 Previous work

Simulating Hamiltonian evolution. Hamiltonian evolution (a.k.a. Schrödinger evolution) is the special case of Eq. (1) where $L_j = 0$ for all j. This simulation problem has received considerable attention since Feynman [12] proposed this as a motivation for building quantum computers; see for example [22, 1, 8, 2, 3, 5, 4, 18, 23, 28, 6]. Some of the recent methods obtain a scaling that is $O(t \operatorname{polylog}(t/\epsilon)\operatorname{poly}(n))$, thereby exceeding what can be accomplished by the longstanding Trotter-Suzuki methods [30].

Simulating Lindblad evolution. The natural generalization from closed systems to Markovian open systems in terms of the Lindblad equation has received much less attention. Kliesch et al. [17] give a quantum algorithm for simulating Lindblad evolution in the case where each of H, L_1, \ldots, L_m can be expressed as a sum of local operators (i.e., which act on a constant number of qubits). The cost of this algorithm with respect to t and ϵ (omitting factors of $\operatorname{poly}(n)$) is $O(t^2/\epsilon)$. Childs and Li [9] improve this to $O(t^{1.5}/\sqrt{\epsilon})$ and also give an $O((t^2/\epsilon)\operatorname{polylog}(t/\epsilon))$ query algorithm for the case where the operators in Eq. (1) are sparse and represented in terms of an oracle. Another result in [9] is an $\Omega(t)$ lower bound for the query complexity for time t when Eq. (1) has H=0 and m=1.

As far as we know, none of the previous algorithms for simulating Lindblad evolution has cost $O(t \operatorname{polylog}(t/\epsilon)\operatorname{poly}(n))$, which is the performance that we attain. Our results are summarized precisely in the next subsection (subsection 1.2).

We note that there are simulation algorithms that solve problems that are related to but different from ours, such as [7], which does not produce the final state; rather it simulates the expectation of an observable applied to the final state. We do not know how to adapt these techniques to produce the unmeasured final state instead.

Finally, we note that there are interesting classical algorithmic techniques for simulating Lindblad evolution that are feasible when the dimension of the Hilbert space (which is 2^n , for n qubits) is not too large—but these do not carry over to the context of quantum algorithms (where n can be large). In the classical setting, since the state is known (and stored) explicitly, various "unravellings" of the process that are state-dependent can be simulated. For example, the random variable corresponding to "the next jump time" (which is highly state-dependent)

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can be simulated. In the context of quantum algorithms, the input state is unknown and cannot be measured without affecting it.

1.2 New results

Eq. (1) can be written as $\dot{\rho} = \mathcal{L}[\rho]$, where \mathcal{L} is a *Lindbladian*, defined as a mapping of the form

$$\mathcal{L}[\rho] = -i[H, \ \rho] + \sum_{j=1}^{m} \left(L_j \rho L_j^{\dagger} - \frac{1}{2} L_j^{\dagger} L_j \rho - \frac{1}{2} \rho L_j^{\dagger} L_j \right), \tag{4}$$

for operators H, L_1, \ldots, L_m on the Hilbert space $\mathcal{H} = \mathbb{C}^{2^n}$ (*n* qubits) with H Hermitian. Evolution under Eq. (1) for time t corresponds to the quantum map $e^{\mathcal{L}t}$ (which is a channel for any $t \geq 0$).

Each of the operators H, L_1, \ldots, L_m corresponds to a $2^n \times 2^n$ matrix. The simulation algorithm is based on a succinct specification of these matrices. Our succinct specification is as a linear combination of q Paulis, defined as

$$H = \sum_{k=0}^{q-1} \beta_{0k} V_{0k} \tag{5}$$

$$L_{j} = \sum_{k=0}^{q-1} \beta_{jk} V_{jk}, \tag{6}$$

where, for each $j \in \{0, ..., m\}$ and $k \in \{0, ..., q-1\}$, V_{jk} is an n-fold tensor product of Paulis $(I, \sigma_x, \sigma_y, \sigma_z)$ and a scalar phase $e^{i\theta}$ $(\theta \in [0, 2\pi])$, and $\beta_{jk} \geq 0$.

In the evolution $e^{\mathcal{L}t}$, it is possible to scale up \mathcal{L} by some factor while reducing t by the same factor, i.e., $e^{\mathcal{L}t}[\rho] = e^{(c\mathcal{L})\frac{t}{c}}[\rho]$ for any $c > 0^1$. This reduces the simulation time but transfers the cost into the magnitude of \mathcal{L} . To normalize this cost, we define a norm based on the specification of \mathcal{L} .

Define the norm² of a specification of a Lindbladian \mathcal{L} as a linear product of Paulis as

$$\|\mathcal{L}\|_{\text{pauli}} = \sum_{k=0}^{q-1} \beta_{0k} + \sum_{j=1}^{m} \left(\sum_{k=0}^{q-1} \beta_{jk}\right)^{2}.$$
 (7)

Our main result is the following theorem.

▶ **Theorem 1.** Let \mathcal{L} be a Lindbladian presented as a linear combination of q Paulis. Then, for any t > 0 and $\epsilon > 0$, there exists a quantum circuit of size

$$O\left(m^2 q^2 \tau \frac{(\log(mq\tau/\epsilon) + n)\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right)$$
(8)

that implements a quantum channel \mathcal{N} , such that $\|\mathcal{N} - e^{\mathcal{L}t}\|_{\diamond} \leq \epsilon$, where $\tau = t \|\mathcal{L}\|_{\mathsf{pauli}}$.

¹ $c\mathcal{L}$ denotes the mapping obtained from \mathcal{L} with H multiplied by c and each L_j multiplied by \sqrt{c} .

² For simplicity we use the terminology $\|\mathcal{L}\|_{\mathsf{pauli}}$ even though the quantity is not directly a function of the mapping \mathcal{L} . However, $\|c\mathcal{L}\|_{\mathsf{pauli}} = c\|\mathcal{L}\|_{\mathsf{pauli}}$ if $c\mathcal{L}$ denotes the expression in Eq. (4) with the factor c multiplied through.

Remarks

- 1. The proof of Theorem 1 is sketched in section 4 and is shown in the full version of this paper [10]. A main novel ingredient of the proof is Lemma 3, concerning a variant of the "linear combination of unitaries" construction that is suitable for channels (explained in sections 2 and 3).
- 2. The factor $\|\mathcal{L}\|_{pauli}$ corresponding to the coefficients of the specification as a linear combination of Paulis is a natural generalization to the case of Lindbladians of a similar factor for Hamiltonians that appears in [3].
- 3. When $m, q \in \text{poly}(n)$, the gate complexity in Theorem 1 simplifies to

$$O\left(\tau \frac{\log(\tau/\epsilon)^2}{\log\log(\tau/\epsilon)}\operatorname{poly}(n)\right). \tag{9}$$

4. A Lindbladian \mathcal{L} is *local* if

$$H = \sum_{j=1}^{m'} H_j, \tag{10}$$

where $H_1, \ldots, H_{m'}$ and also L_1, \ldots, L_m are local (i.e., they each act on a constant number of qubits). A *local* specification of \mathcal{L} is as $H_1, \ldots, H_{m'}, L_1, \ldots, L_m$ and we define its norm

$$\|\mathcal{L}\|_{\text{local}} = \sum_{j=1}^{m'} \|H_j\| + \sum_{j=1}^{m} \|L_j\|^2.$$
(11)

For local Lindbladians, Theorem 1 reduces to the following.

▶ Corollary 2. If \mathcal{L} is a local Lindbladian then the gate complexity for simulating $e^{\mathcal{L}t}$ with precision ϵ is

$$O\left(\left(m+m'\right)\tau \frac{\log(\left(m+m'\right)\tau/\epsilon)\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right),\tag{12}$$

where $\tau = t \|\mathcal{L}\|_{local}$.

5. We also consider sparse Lindbladians (see [9] for various definitions, extending definitions and specifications of sparse Hamiltonians [1]). Here, we define a Lindbladian to have d-sparse operators if H, L_1, \ldots, L_m each have at most d non-zero entries in each row/column. A sparse specification of such a Lindbladian \mathcal{L} is as a black-box that provides the positions and values of the non-zero entries of each row/column of H, L_1, \ldots, L_m via queries. Define the norm of any specification of a Lindbladian in terms of operators H, L_1, \ldots, L_m as

$$\|\mathcal{L}\|_{\mathsf{ops}} = \|H\| + \sum_{j=1}^{m} \|L_j\|^2.$$
 (13)

The query complexity and gate complexity for simulating d-sparse Lindbladians \mathcal{L} are

$$O(\tau \operatorname{polylog}(mq\tau/\epsilon)\operatorname{poly}(d,n)),$$
 (14)

where $\tau = t \|\mathcal{L}\|_{\text{ops}}$. We sketch the analysis in the full version of this paper [10].

6. We expect some of the methodologies in [3, 4, 23, 28] to be adaptable to the Lindblad evolution simulation problem (in conjunction with our variant of the LCU construction and oblivious amplitude amplification), but have not investigated this.

2 Brief summary of novel techniques

As noted in subsection 1.1, for the case of Hamiltonian evolution, a series of recent quantum algorithms whose scaling is $O(t \operatorname{polylog}(t/\epsilon))$ have been discovered which improve on what has been accomplished using the longstanding Trotter-Suzuki decomposition. One of the main tools that these algorithms employ is a remarkable circuit construction that is based on a certain decomposition of unitary operations (or near-unitary operations) into a linear combination of unitaries. We refer to this construction as the standard LCU method.

For the case of Lindblad evolution, the operations that arise are channels that are not generally unitary. Some channels are mixed unitary, which means that they can be expressed as a randomly chosen unitary (say with probabilities p_0, \ldots, p_{m-1} on the unitaries U_0, \ldots, U_{m-1}). For such channels, the standard LCU method can be adapted along the lines of first randomly sampling $j \in \{0, \ldots, m-1\}$ and then applying the standard LCU method to the unitary U_j . However, there exist channels that are not mixed unitary—and such channels can arise from the Lindblad equation. A different reductionist approach is to express these channels in the Stinespring form, as unitary operations that act on a larger system, and then apply the standard LCU method to those unitaries; however, as we explain in subsection 2.1, this approach performs poorly. We take a different approach that does not involve a reduction to the unitary case: we have developed a new variant of the LCU method that is for channels. This is explained in section 3.

Another new technique that we employ is an Oblivious Amplitude Amplification algorithm for isometries (as opposed to unitaries), which is noteworthy because a reductionist approach based on extending isometries to unitaries does not work. Roughly speaking, this is because our LCU construction turns out to produce an isometry (corresponding to a purification of the channel); however, it does not produce a unitary extension of that isometry.

2.1 The standard LCU method performs poorly on Stinespring dilations

Here we show in some technical detail why the standard LCU method performs poorly for Stinespring dilations of channels. The standard LCU method (explained in detail in Sec. 2.1 of [18]) for a unitary V expressible as a linear combination of unitaries as $V = \alpha_0 U_0 + \cdots + \alpha_{m-1} U_{m-1}$ is a circuit construction W that has the property

$$W|0\rangle|\psi\rangle = \sqrt{p}|0\rangle V|\psi\rangle + \sqrt{1-p}|\Phi^{\perp}\rangle \tag{15}$$

where $|\Phi^{\perp}\rangle$ has zero amplitude in states with first register $|0\rangle$ (i.e., $(|0\rangle\langle 0| \otimes I)|\Phi^{\perp}\rangle = 0$) and

$$p = \frac{1}{(\sum_{i=0}^{m-1} \alpha_i)^2} \tag{16}$$

is the success probability (that arises if the first indicator register is measured).

Consider the *amplitude damping channel*, which has two Kraus operators with the following LCU decompositions

$$A_{0} = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1 - \delta} \end{bmatrix} = \alpha_{00} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \alpha_{01} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$A_{1} = \begin{bmatrix} 0 & \sqrt{\delta} \\ 0 & 0 \end{bmatrix} = \alpha_{10} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \alpha_{11} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

where $\alpha_{00} = \frac{1+\sqrt{1-\delta}}{2}$, $\alpha_{01} = \frac{1-\sqrt{1-\delta}}{2}$, $\alpha_{10} = \frac{\sqrt{\delta}}{2}$, $\alpha_{11} = \frac{\sqrt{\delta}}{2}$. Evolving an amplitude damping process for time t yields this channel with $\delta = 1 - e^{-t}$. When $t \ll 1$, $\delta \approx t$, $\alpha_{00} \approx 1 - t/4$, and $\alpha_{01} \approx t/4$.

A Stinespring dilation of V and its LCU decomposition can be derived from the above LCU decompositions of A_0 and A_1 as

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{1-\delta} & -\sqrt{\delta} & 0 \\ 0 & \sqrt{\delta} & \sqrt{1-\delta} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \alpha_{00} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \alpha_{01} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \alpha_{11} \begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \alpha_{11} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}.$$

Applying the standard LCU method here results in a success probability (computed from Eq. (16)) of

$$\frac{1}{\left(\alpha_{00} + \alpha_{01} + \alpha_{10} + \alpha_{11}\right)^2} = \frac{1}{\left(1 + \sqrt{\delta}\right)^2} = 1 - 2\sqrt{\delta} + \Theta(\delta).$$

For small time evolution t, the failure probability is $\Theta(\sqrt{t})$, which is prohibitively expensive. It means that the process can be repeated at most $\Theta(1/\sqrt{t})$ times until the cumulative failure probability becomes a constant. The amount of evolution time (of the amplitude damping process) that this corresponds to is

$$\Theta\left(\frac{1}{\sqrt{t}}\right) \cdot t = \Theta(\sqrt{t}),$$

which is subconstant as $t \to 0$. This creates a problem in the general Lindblad simulation.

Our new LCU method for channels (explained in section 3) achieves the higher success probability

$$\frac{1}{(\alpha_{00} + \alpha_{01})^2 + (\alpha_{10} + \alpha_{11})^2} = \frac{1}{1+\delta} = 1 - \delta + \Theta(\delta^2).$$

For small time evolution t, the failure probability is $\Theta(t)$. Now, the process can be repeated $\Theta(1/t)$ times until the cumulative failure probability becomes a constant, which corresponds to evolution time

$$\Theta\left(\frac{1}{t}\right) \cdot t = \Theta(1),$$

which is constant as $t \to 0$. Since this is consistent with what arises in the algorithm of simulating Hamiltonian evolution in [2, 3], the methodologies used therein, with various adjustments, can be used to obtain the simulation bounds.

3 New LCU method for channels and completely positive maps

Let A_0, \ldots, A_{m-1} , linear operators on \mathbb{C}^{2^n} (*n*-qubit states), be the Kraus operators of a channel. Suppose that, for each $j \in \{0, \ldots, m-1\}$, we have a decomposition of A_j as a linear combination of unitaries in the form

$$A_{j} = \sum_{k=0}^{q-1} \alpha_{jk} U_{jk}, \tag{17}$$

Figure 2 The circuit W for simulating a channel using the new LCU method.

where, for each $j \in \{0, ..., m-1\}$ and $k \in \{0, ..., q-1\}$, $\alpha_{jk} \geq 0$ and U_{jk} is unitary.

The objective is to implement the channel in terms of the implementations of U_{jk} 's. We will describe a circuit W and fixed state $|\mu\rangle$ such that, for any n-qubit state $|\psi\rangle$,

$$W|0\rangle|\mu\rangle|\psi\rangle = \sqrt{p}|0\rangle \left(\sum_{j=0}^{m-1} |j\rangle A_j|\psi\rangle\right) + \sqrt{1-p}|\Phi^{\perp}\rangle, \tag{18}$$

where $(|0\rangle\langle 0|\otimes I\otimes I)|\Phi^{\perp}\rangle = 0$ and

$$p = \frac{1}{\sum_{j=0}^{m-1} (\sum_{k=0}^{q-1} \alpha_{jk})^2}$$
 (19)

is called the success probability parameter (which is realized if the first register is measured). Note that the isometry $|\psi\rangle\mapsto\sum_{j=0}^{m-1}|j\rangle A_j|\psi\rangle$ is the channel in purified form.

The circuit W is in terms of two gates. One gate is a multiplexed-U gate, denoted by multi-U such that, for all $j \in \{0, \ldots, m-1\}$ and $k \in \{0, \ldots, q-1\}$,

$$\operatorname{multi-}U|k\rangle|j\rangle|\psi\rangle = |k\rangle|j\rangle U_{ik}|\psi\rangle. \tag{20}$$

The other gate is a multiplexed-B gate, denoted by multi-B, such that, for all $j \in \{0, ..., m-1\}$,

$$\text{multi-}B|0\rangle|j\rangle = \left(\frac{1}{\sqrt{s_j}} \sum_{k=0}^{q-1} \sqrt{\alpha_{jk}}|k\rangle\right)|j\rangle,\tag{21}$$

where

$$s_j = \sum_{k=0}^{q-1} \alpha_{jk}.$$
 (22)

Define the state $|\mu\rangle$ (in terms of s_0, \ldots, s_{m-1} from Eq. (22))

$$|\mu\rangle = \frac{1}{\sqrt{\sum_{j=1}^{m-1} s_j^2}} \sum_{j=0}^{m-1} s_j |j\rangle.$$
 (23)

Define the circuit W (acting on $\mathbb{C}^q \otimes \mathbb{C}^m \otimes \mathbb{C}^{2^n}$) as

$$W = (\text{multi-}B^{\dagger} \otimes I)\text{multi-}U(\text{multi-}B \otimes I). \tag{24}$$

The LCU construction with the circuit W with its initial state $|0\rangle \otimes |\mu\rangle \otimes |\psi\rangle$ is illustrated in Fig. 2.

In this figure, we refer to the first register as the *indicator register* (as it indicates whether the computation succeeds at the end of this operation), the second register as the *purifier*

register (as it is used to purify the channel when the computation succeeds), and the third register as the system register (as it contains the state being evolved).

In the following lemma, Eq. (18) is shown to apply where A_0, \ldots, A_{m-1} are arbitrary linear operators (i.e., Kraus operators of a completely positive map that is not necessarily trace preserving). If the map is also trace preserving then $\sum_{j=0}^{m-1} |j\rangle A_j |\psi\rangle$ and $|\Phi^{\perp}\rangle$ are normalized states and the success probability parameter p is the actual success probability realized if the first register is measured; otherwise, these need not be the case. In subsequent sections, we will apply this lemma in a context where the trace preserving condition is approximately satisfied.

▶ Lemma 3. Let A_0, \ldots, A_{m-1} be the Kraus operators of a completely positive map. Suppose that each A_j can be written in the form of Eq. (17). Let multi-U, multi-B, W, and $|\mu\rangle$ be defined as above. Then applying the unitary operator W on any state of the form $|0\rangle|\mu\rangle|\psi\rangle$ produces the state

$$\sqrt{p}|0\rangle \left(\sum_{j=0}^{m-1}|j\rangle A_j|\psi\rangle\right) + \sqrt{1-p}|\Phi^{\perp}\rangle,$$

where $(|0\rangle\langle 0|\otimes I\otimes I)|\Phi^{\perp}\rangle = 0$, and

$$p = \frac{1}{\sum_{j=0}^{m-1} \left(\sum_{k=0}^{q-1} \alpha_{jk}\right)^2} .$$

Proof. First consider the state $|0\rangle|j\rangle|\psi\rangle$ for any $j \in \{0, ..., m-1\}$. Applying W on this state is the standard LCU method [18]:

$$W|0\rangle|j\rangle|\psi\rangle = (\text{multi-}B^{\dagger} \otimes I)\text{multi-}U(\text{multi-}B \otimes I)|0\rangle|j\rangle|\psi\rangle$$
(25)

$$= \frac{1}{\sqrt{s_j}} (\text{multi-}B^{\dagger} \otimes I) \text{multi-}U \left(\sum_{k=0}^{q-1} \sqrt{\alpha_{jk}} |k\rangle \right) |j\rangle |\psi\rangle$$
 (26)

$$= \frac{1}{\sqrt{s_j}} (\text{multi-}B^{\dagger} \otimes I) \left(\sum_{k=0}^{q-1} \sqrt{\alpha_{jk}} |k\rangle |j\rangle U_{jk} |\psi\rangle \right)$$
 (27)

$$= \frac{1}{s_j} |0\rangle |j\rangle \left(\sum_{k=0}^{q-1} \alpha_{jk} U_{jk} |\psi\rangle \right) + \sqrt{\gamma_j} |\Phi_j^{\perp}\rangle$$
 (28)

$$= \frac{1}{s_j} |0\rangle |j\rangle A_j |\psi\rangle + \sqrt{\gamma_j} |\Phi_j^{\perp}\rangle, \tag{29}$$

where $|\Phi_j^{\perp}\rangle$ is a state satisfying $(|0\rangle\langle 0|\otimes I\otimes I)|\Phi_j^{\perp}\rangle=0$ and γ_j is some normalization factor. Up to this point, if the indicator register were measured and $|0\rangle$ were observed as the "success" case as in the standard LCU method, then the state of the purifier and the system register collapses to $|j\rangle A_j|\psi\rangle$. However, this is not a meaningful quantum sate, as it only captures one Kraus operator of a quantum map. Now we use this specially designed quantum state $|\mu\rangle$ to obtain the desired purification state. We use the superposition $|\mu\rangle$ instead of $|j\rangle$ in the second register then, by linearity, we have

$$W|0\rangle|\mu\rangle|\psi\rangle = \sqrt{p}|0\rangle \left(\sum_{j=0}^{m-1} |j\rangle A_j|\psi\rangle\right) + \sqrt{1-p}|\Phi^{\perp}\rangle, \tag{30}$$

where
$$(|0\rangle\langle 0|\otimes I\otimes I)|\Phi^{\perp}\rangle = 0$$
 and $p = \frac{1}{\sum_{j=0}^{m-1} s_j^2}$.

4 Overview of the main result, Theorem 1

In this section we briefly sketch how to apply our new LCU method in order to prove our main result, Theorem 1. The overall structure is similar to that in [2] and [3], with the main novel ingredient being our variant of the LCU construction (explained in section 3) and also a variant of oblivious amplitude amplification for isometries. For clarity, the details are organized into section 4 of the full version of this paper [10], whose content is summarized as:

- 1. In Sec. 4.1 of [10], we describe a simple mapping \mathcal{M}_{δ} in terms of Kraus operators that are based on the operators in \mathcal{L} . For small δ , \mathcal{M}_{δ} is a good approximation of $e^{\mathcal{L}\delta}$.
- 2. In Sec. 4.2 of [10], we show how to simulate the mapping \mathcal{M}_{δ} in the sense of Lemma 3, with success probability parameter $1 O(\delta)$.
- 3. In Sec. 4.3 of [10], we show how to combine r simulations of $\mathcal{M}_{O(1/r)}$ so as to obtain cumulative success probability parameter 1/4. Conditional on success, this produces a good approximation of constant-time Lindblad evolution.
- 4. In Sec. 4.4 of [10], we show how to apply a modified version of oblivious amplitude amplification to unconditionally simulate an approximation of constant-time Lindblad evolution.
- **5.** In Sec. 4.5 of [10], we show how to reduce the number of multiplexed Pauli gates by a concentration bound on the amplitudes associated with nontrivial Pauli gates.
- **6.** In Sec. 4.6 of [10], we bound the total number of gates and combine the simulations for segments in order to complete the proof of Theorem 1.

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- References

- 1 D. Aharonov and A. Ta-Shma. Adiabatic quantum state generation and statistical zero knowledge. In *Proceedings of the 35th ACM Symposium on Theory of Computing*, pages 20–29, 2003. doi:10.1145/780542.780546.
- D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma. Exponential improvement in precision for simulating sparse Hamiltonians. In *Proceedings of the 46th ACM Symposium on Theory of Computing*, pages 283–292, 2014. arXiv:arXiv:1312.1414, doi:10.1145/2591796.2591854.
- 3 D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma. Simulating Hamiltonian dynamics with a truncated Taylor series. *Phys. Rev. Lett.*, 114:090502, Mar 2015. doi: 10.1103/PhysRevLett.114.090502.
- 4 D. W. Berry, A. M. Childs, and R. Kothari. Hamiltonian simulation with nearly optimal dependence on all parameters. In *Proceedings of FOCS 2015*, 2015. arXiv:arXiv:1501. 01715.
- 5 D. W. Berry, R. Cleve, and S. Gharibian. Gate-efficient discrete simulations of continuous-time quantum query algorithms. *Quantum Information and Computation*, 14(1-2):1-30, 2014. arXiv:arXiv:1211.4637.
- 6 D. W. Berry and L. Novo. Corrected quantum walk for optimal Hhamiltonian simulation, 2016. arXiv:1606.03443.
- 7 R. Di Candia, J. S. Pedernales, A. del Campo, E. Solano, and J. Casanova. Quantum simulation of dissipative processes without reservoir engineering. *Sci. Rep.*, 5:9981, 2015.
- 8 A. M. Childs. Quantum information processing in continuous time. PhD thesis, Massachusetts Institute of Technology, 2014.

- 9 A. M. Childs and T. Li. Efficient simulation of sparse markovian quantum dynamics, 2016. arXiv:1611.05543.
- Richard Cleve and Chunhao Wang. Efficient quantum algorithms for simulating lindblad evolution. arXiv preprint arXiv:1612.09512, 2016.
- 11 R. Dorner, J. Goold, and V. Vedral. Towards quantum simulations of biological information flow. *Interface focus*, page rsfs20110109, 2012.
- 12 R. P. Feynman. Simulating physics with computers. *International Journal of Theoretical Physics*, 21(6–7):467–488, 1982.
- V. Gorini, A. Kossakowski, and E. C. G. Sudarshan. Completely positive dynamical semigroups of n-level systems. *Journal of Mathematical Physics*, 17:821–825, 1976.
- 14 S. F. Huelga and M. B. Plenio. Vibrations, quanta and biology. *Contemporary Physics*, 54(4):181–207, 2013.
- 15 M. J. Kastoryano and F. G. S. L. Brandao. Quantum gibbs samplers: the commuting case. Communications in Mathematical Physics, 344(3):915–957, 2016.
- 16 M. J. Kastoryano, F. Reiter, and A. S. Sørensen. Dissipative preparation of entanglement in optical cavities. *Physical review letters*, 106(9):090502, 2011.
- 17 M. Kliesch, T. Barthel, C. Gogolin, M. Kastoryano, and J. Eisert. Dissipative quantum church-turing theorem. *Physical review letters*, 107(12):120501, 2011.
- 18 R. Kothari. Efficient algorithms in quantum query complexity. PhD thesis, University of Waterloo, 2014.
- 19 B. Kraus, H.P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller. Preparation of entangled states by quantum markov processes. *Physical Review A*, 78(4):042307, 2008.
- 20 A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger. Dynamics of the dissipative two-state system. Reviews of Modern Physics, 59(1):1, 1987.
- 21 G. Lindblad. On the generators of quantum dynamical systems. *Communications in Mathematical Physics*, 48:119–130, 1976.
- 22 S. Lloyd. Universal quantum simulators. *Science*, 273(5278):1073–1078, 1996.
- 23 G. H. Low and I. L. Chuang. Optimal Hamiltonian simulation by quantum signal processing, 2016. arXiv:1606.02685.
- 24 E. Magesan, D. Puzzuoli, C. E. Granade, and D. G. Cory. Modeling quantum noise for efficient testing of fault-tolerant circuits. *Physical Review A*, 87(1):012324, 2013.
- V. May and O. Kühn. Charge and energy transfer dynamics in molecular systems. John Wiley & Sons, 2008.
- S. Mostame, P. Rebentrost, A. Eisfeld, A. J. Kerman, D. I. Tsomokos, and A. Aspuru-Guzik. Quantum simulator of an open quantum system using superconducting qubits: exciton transport in photosynthetic complexes. New Journal of Physics, 14(10):105013, 2012.
- 27 A. Nitzan. Chemical dynamics in condensed phases: relaxation, transfer and reactions in condensed molecular systems. Oxford university press, 2006.
- A. Patel and A. Priyadarsini. Optimization of quantum hamiltonian evolution: from two projection operators to local hamiltonians. *International Journal of Quantum Information*, page 1650027, 2016.
- **29** F. Reiter, D. Reeb, and A.S. Sørensen. Scalable dissipative preparation of many-body entanglement. *Physical Review Letters*, 117(4):040501, 2016.
- 30 M. Suzuki. General theory of fractal path integrals with applications to many-body theories and statistical physics. *Journal of Mathematical Physics*, 32(2):400–407, 1991.
- 31 F. Verstraete, M. M. Wolf, and J. I. Cirac. Quantum computation and quantum-state engineering driven by dissipation. *Nature physics*, 5(9):633–636, 2009.
- 32 U. Weiss. Quantum dissipative systems. World scientific, 2012.

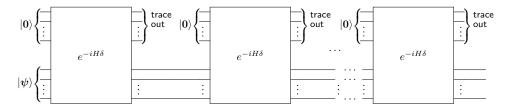


Figure 3 N-stage ϵ -precision discretization of the trajectory resulting from \mathcal{L} . For each $k \in \{1, ..., N\}$, after k stages, the channel should be within ϵ of $\exp\left(\frac{kT}{N}\mathcal{L}\right)$.

A Cost of expressing Lindblad evolution as Hamiltonian evolution

Let \mathcal{L} be a Lindbladian acting on an n-qubit register \mathcal{H} over a time interval [0,T]. For each initial state, \mathcal{L} associates a trajectory, consisting of a density operator $\rho(t)$ for each $t \in [0,T]$. Here we show that if this is simulated by Hamiltonian evolution in a larger system with an ancillary register that is continually reset (expressed as a limiting case when $N \to \infty$ in the process illustrated in Figure 3) then the total evolution time for this Hamiltonian can be necessarily infinite.

▶ Definition 4. Define an N-stage ϵ -precision discretization of \mathcal{L} for interval [0,T] as an ancillary register \mathcal{K} , a Hamiltonian H (with ||H||=1) acting on the joint system $\mathcal{K} \otimes \mathcal{H}$, and $\delta \geq 0$ such that the channel $\mathcal{N}_{H\delta}$ defined as

$$\mathcal{N}_{H\delta}[\rho] = \text{Tr}_{\mathcal{K}}(e^{-iH\delta}(|0\rangle\langle 0| \otimes \rho)e^{iH\delta})$$
(31)

has the following property. $\mathcal{N}_{H\delta}$ approximates evolution under \mathcal{L} in the sense that, for each $j \in \{1, \ldots, N\}$,

$$\left\| \left(\mathcal{N}_{H\delta} \right)^k - \exp\left(\frac{kT}{N} \mathcal{L} \right) \right\|_{\alpha} \le \epsilon. \tag{32}$$

That is, the N points generated by $\mathcal{N}_{H\delta}$, $(\mathcal{N}_{H\delta})^2$, ..., $(\mathcal{N}_{H\delta})^N$ approximate the corresponding points on the trajectory determined by \mathcal{L} .

Our lower bound is for the amplitude damping process on a 1-qubit system is the time-evolution described by the Lindbladian \mathcal{L} , where

$$\mathcal{L}[\rho] = L\rho L^{\dagger} - \frac{1}{2}(L^{\dagger}L\rho + \rho L^{\dagger}L), \tag{33}$$

and
$$L = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
.

▶ Theorem 5. Any $\frac{1}{4}$ -precision N-stage approximation of the amplitude damping process over the time interval $[0, \ln 2]$ has the property that the total evolution time of H is $\Omega(\sqrt{N})$. (Note that this lower bound is independent of the dimension of the ancillary system.)

To prove Theorem 5, we first prove the following Local Hamiltonian Approximation lemma. This concerns a scenario where H is a Hamiltonian acting on a joint system of two registers, a system register \mathcal{H} and an ancillary register \mathcal{K} , and where \mathcal{K} is traced out after this evolution. Informally, the lemma states that, if the initial state is a product state and the evolution time is short, then this process can be approximated by the evolution of another Hamiltonian G that acts on \mathcal{H} alone. This is illustrated in figure 4.



- Figure 4 The Local Hamiltonian Approximation Lemma. The first register is d-dimensional, the second register contains n qubits, and the approximation is within $O(\delta^2)$ (independent of d and n).
- ▶ Lemma 6 (Local Hamiltonian approximation). Let \mathcal{H} be an n-qubit register and \mathcal{K} a d-dimensional register. Let H be a Hamiltonian (with ||H|| = 1) acting on the joint system $\mathcal{K} \otimes \mathcal{H}$. Define the n-qubit channel $\mathcal{N}_{H\delta}$ as

$$\mathcal{N}_{H\delta}[\rho] = \text{Tr}_{\mathcal{K}} \left(e^{-iH\delta} (|0\rangle\langle 0| \otimes \rho) e^{iH\delta} \right). \tag{34}$$

Then there exists a Hamiltonian G (with ||G|| = 1), acting on \mathcal{H} alone, such that $\mathcal{N}_{G\delta}$ defined as

$$\mathcal{N}_{G\delta}[\rho] = e^{-iG\delta}\rho \,e^{iG\delta} \tag{35}$$

satisfies $\|\mathcal{N}_{H\delta} - \mathcal{N}_{G\delta}\|_1 \in O(\delta^2)$. (The notation $\|\cdot\|_1$ indicates the trace-induced norm, which is sufficient for our purposes because our application is a lower bound.)

Proof. Viewing H as a $d \times d$ block matrix, we have

$$H = \sum_{j=0}^{d-1} \sum_{k=0}^{d-1} |j\rangle\langle k| \otimes H_{jk}$$

$$\tag{36}$$

and we refer to H_{jk} as the (j,k) block. Define D as the diagonal blocks of H, namely

$$D = \sum_{j=0}^{d-1} |j\rangle\langle j| \otimes H_{jj}, \tag{37}$$

and set J = H - D (the off-diagonal blocks). Note that $||D||, ||J|| \le 1$ and $||e^{-iH\delta} - e^{-iD\delta}e^{-iJ\delta}|| \le \delta^2$, for $\delta > 0$, which permits us to consider the effect of J and D separately.

Now consider the state $e^{-iJ\delta}|0\rangle\otimes|\psi\rangle$. We will show that, if the measurement corresponding to projectors $|0\rangle\langle 0|$ and $I-|0\rangle\langle 0|$ is performed on register \mathcal{K} , then the residual state has trace distance $O(\delta^2)$ from $|0\rangle\otimes|\psi\rangle$. Since the (0,0) block of J is 0,

$$J\delta |0\rangle \otimes |\psi\rangle = \delta' |\Psi^{\perp}\rangle, \tag{38}$$

where $|\Psi^{\perp}\rangle$ is a state such that $(|0\rangle\langle 0|\otimes I)|\Psi^{\perp}\rangle = 0$ and $0 \leq \delta' \leq \delta$. Therefore,

$$e^{-iJ\delta}|0\rangle\otimes|\psi\rangle = \sum_{r=0}^{\infty} \frac{(-iJ\delta)^r}{r!}|0\rangle\otimes|\psi\rangle$$
 (39)

$$= |0\rangle \otimes |\psi\rangle - i\delta' |\Psi^{\perp}\rangle + \delta'' |\Phi\rangle, \tag{40}$$

where $0 \le \delta'' \le e^{\delta} - 1 - \delta \in O(\delta^2)$. It follows that, if the above measurement is performed on register \mathcal{K} , then the probability of measurement outcome $I - |0\rangle\langle 0|$ is at most $(\delta')^2 + (\delta'')^2 \in O(\delta^2)$. This implies that the state when register \mathcal{K} of $e^{-iJ\delta}|0\rangle \otimes |\psi\rangle$ is traced out, namely

$$\operatorname{Tr}_{\mathcal{K}}\left(e^{-iJ\delta}(|0\rangle\langle 0|\otimes |\psi\rangle\langle \psi|)e^{iJ\delta}\right),\tag{41}$$

has trace distance $O(\delta^2)$ from the original state $|\psi\rangle\langle\psi|$.

Therefore, for states of the form $|0\rangle \otimes |\psi\rangle$, the operation $e^{-iH\delta}$ can be approximated by $e^{-iD\delta}$ at the cost of an error of $O(\delta^2)$ in trace distance. The result follows by setting $G = H_{00}$ (the (0,0) block of D).

17:14 Efficient Quantum Algorithms for Simulating Lindblad Evolution

Proof of Theorem 5. It is straightforward to check that, starting with the initial state $|1\rangle\langle 1|$ and evolving by the amplitude damping process for time $T = \ln 2$ produces the maximally mixed state.

Consider any $\frac{1}{4}$ -precision N-stage discretization of this process, with Hamiltonian H and $\delta > 0$. We can apply the Local Hamiltonian Approximation Lemma (Lemma 6) to approximate each of the N evolutions of H with evolution by a Hamiltonian G that is local to the qubit. The result is unitary evolution of the qubit that approximates the amplitude damping process within trace distance error at most $O(N\delta^2)$.

Unitary evolution applied to $|1\rangle\langle 1|$ results in a pure state, and the trace distance between any pure state and the maximally mixed state is $\frac{1}{2}$. Therefore, to avoid a contradiction, we must have $N\delta^2 \in \Omega(1)$, which implies that $\delta \in \Omega(1/\sqrt{N})$. Therefore, the total evolution time of H is $N\delta \in \Omega(\sqrt{N})$.