Quantum simulation of the Lindblad equation using a unitary decomposition of operators

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(Received 13 November 2021; accepted 19 April 2022; published 15 June 2022)

Accurate simulation of the time evolution of a quantum system under the influence of an environment is critical to making accurate predictions in chemistry, condensed-matter physics, and materials sciences. Whereas there has been a recent surge in interest in quantum algorithms for the prediction of nonunitary time evolution in quantum systems, few studies offer a direct quantum analog to the Lindblad equation. Here, we present a quantum algorithm—utilizing a decomposition of nonunitary operators approach—that models dynamic processes via the unraveled Lindblad equation. This algorithm is employed to probe both a two-level system in an amplitude damping channel as well as the transverse field Ising model in a variety of parameter regimes; the resulting population dynamics demonstrate excellent agreement with classical simulation, showing the promise of predicting population dynamics utilizing quantum devices for a variety of important systems in molecular energy transport, quantum optics, and other open quantum systems.

DOI: 10.1103/PhysRevResearch.4.023216

I. INTRODUCTION

Emerging quantum technologies have recently generated interest in open quantum system (OQS) methods that predict environmentally driven dynamics because of the environmental interactions inherent in quantum hardware. Classically, a plethora of methods has been developed to treat the dynamics of open quantum systems, including master equation approaches and numerically exact methods [1]. Another widely used class of OQS methods relies on the reduced density matrix formalism where the environmental degrees of freedom are integrated out with a master equation being utilized to treat the subsystem dynamics under the influence of an environment. Two commonly used master equation approaches are Redfield [2] and Gorini–Kossakowski–Sudarshan–Lindblad [3,4], with the latter being derived from the completely positive Kraus map formulation and, hence, retaining the positivity of the system density matrix. As the positivity of the reduced density matrix relates to the probability of finding an electron in a given state, positivity is required for the reduced density matrix to retain physical meaning or N representability [5–8]. This formalism has also been adapted for the treatment of accurate fermionic statistics [9] and for non-Markovian dynamics [10,11]. The Lindblad formalism has proven to be a powerful tool in predicting the dynamics of a variety of open quantum system dynamics under the Born-Markov approximation in quantum optics [12], quantum transport [13], excitonic energy transport [14–19], and spin dynamics [20–23].

In recent years, substantial progress has been made in quantum computation in terms of both hardware and algorithm development. Noisy intermediate-scale quantum (NISQ) computers are now publicly accessible, allowing for the recent explosion of quantum computing studies with considerable work being dedicated to using these devices to model, probe, and solve physically relevant problems [24–30]. In quantum chemistry, these devices have been used to make predictions in materials, periodic systems [31–34], as well as many molecular properties including electron correlation [35,36], ground-state energies [37–42], and excited-state energies [43–46]. Moreover, research has been dedicated to using quantum devices to predict superconductivity and long-range order [47,48] as well as create excitonic condensates [49]. The biggest challenge faced by these hardware platforms continues to be the detrimental effects of environmental noise [50,51], thus, limiting the scope and size of problems that can be tackled on NISQ hardware.

There has been a recent surge in interest in using quantum computers to model and predict the dynamics of open quantum systems. Whereas mapping the inherently nonunitary dynamics into the unitary framework of gate-based quantum algorithms presents challenges, much progress has been made towards this goal [52–55]. Examples include algorithms based on imaginary-time evolution [56–58], the time-dependent variational principle [59], and duality quantum algorithms [60,61]. A popular method of approach is through explicit dilation, taking the nonunitary dynamics and mapping them into a larger Hilbert space where they become unitary [62–67]. Whereas these methods have shown to be efficient for several test systems in a variety of regimes of dynamics, they are restricted by the requirement that the evolving map must be a contraction mapping. We presented an alternative approach

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that relies on the basic decomposition of any evolving operator bypassing the requirement of utilizing contraction mappings [54]. However, most of this previous work has relied on the Kraus operator formalism [54,62,63,65–67], which can be limited because the Kraus operators are not always known. Lindbladian operators are often better known and more physically motivated, making algorithms that can work directly with the Lindblad equation appealing. Despite its success in classical simulation, to date there have been few studies dedicated to the development of a robust quantum algorithm directly analogous to the Lindblad equation [57].

In this *paper* we develop an algorithm using Lindbladian operators directly, instead of utilizing the Kraus framework as was shown in previous work [54]. We demonstrate this algorithm on a two-level system in an amplitude damping channel and on the transverse field Ising model in different parameter regimes. The close agreement with classical simulation demonstrates the promise of such a unitary decomposition of Lindbladian operators with this algorithm having potentially far reaching applicability to problems in quantum chemistry, physics, and control theory.

II. THEORY AND METHODS

The Lindblad equation describes the dynamics of an open quantum system under the Born-Markov approximation,

$$\frac{d\rho}{dt} = -i[\hat{H}, \rho] + \sum_k \gamma_k \left(\hat{C}_k \rho \hat{C}_k^\dagger - \frac{1}{2}\{\hat{C}_k^\dagger \hat{C}_k, \rho\} \right), \quad (1)$$

where ρ is the system density matrix, $\hat{H}$ is the system Hamiltonian, γ_k is the decay rate, $\hat{C}_k$s are the Lindbladian operators, and the summation is over k channels of environmental interaction [1,3,4]. The Lindbladian operators are often physically motivated, which combined with the guaranteed positivity makes this master equation form quite powerful.

Another way of writing the Lindblad equation is in the vectorized form, also called the unraveled master equation (UME),

$$\frac{d|\rho\rangle}{dt} = \hat{\mathcal{L}}|\rho\rangle, \quad (2)$$

with,

$$\hat{\mathcal{L}} = -i\mathbb{I} \otimes \hat{H} + i\hat{H}^T \otimes \mathbb{I} + \sum_k \hat{C}_k^* \otimes \hat{C}_k - \frac{1}{2}\mathbb{I} \otimes (\hat{C}_k^\dagger \hat{C}_k) - \frac{1}{2}\hat{C}_k^T \hat{C}_k^* \otimes \mathbb{I}, \quad (3)$$

where the superscripts $*, T$, and $\dagger$ represent the complex conjugate, transpose, and adjoint operators, respectively, $|\rho\rangle$ is the vectorized density matrix, and $\hat{\mathcal{L}}$ is the Lindbladian superoperator generating the dynamics [68]. This form of the Lindblad equation can be directly integrated where the time propagator is given by

$$|\rho(t)\rangle = e^{\hat{\mathcal{L}}t}|\rho(0)\rangle. \quad (4)$$

The vectorization operator is defined by stacking the columns of ρ resulting in a column vector,

$$|\rho\rangle = \mathrm{vec}(\rho) = \begin{pmatrix} \rho_{00} \\ \rho_{10} \\ \vdots \\ \rho_{nn} \end{pmatrix}. \quad (5)$$

If the density matrix is size m, then the vectorized density matrix will be length m^2.

In general the propagator in Eq. (4) is nonunitary, and we implement this exponential operator as a sum of unitary operators. The vectorized Lindblad equation has been used to study systems, such as non-Hermitian Hamiltonians and dissipations [69], spontaneous emission [70], and Ising models [57].

In order to implement this nonunitary propagation on a quantum circuit, we decompose the operator into unitary components. As shown in previous work, any operator can be decomposed into Hermitian and anti-Hermitian components through the relation,

$$\hat{M} = \hat{S} + \hat{A}, \quad (6)$$

where $\hat{S}$ is a Hermitian operator and $\hat{A}$ is an anti-Hermitian operator [54]. In the context of the unraveled master equation, we define $\hat{M} = e^{\hat{\mathcal{L}}t}$ and simulate the entire dynamics using one operator and one quantum circuit, whereas previously we decomposed each Kraus operator individually. $\hat{S}$ and $\hat{A}$ are approximated using first-order Taylor expansions in an expansion parameter ϵ,

$$\hat{S} = \lim_{\epsilon \to 0} \frac{1}{2\epsilon}(ie^{-i\epsilon\hat{S}} - ie^{i\epsilon\hat{S}})$$
$$\hat{A} = \lim_{\epsilon \to 0} \frac{1}{2\epsilon}(e^{\epsilon\hat{A}} - e^{-\epsilon\hat{A}}). \quad (7)$$

Both the Hermitian and the anti-Hermitian operators have been written in terms of unitaries. The operators have error $O(\epsilon^2)$, and the error can be systematically improved with Richardson extrapolation [54,71].

The propagation can be performed with unitary gates on a dilated space by

$$\hat{R}\hat{U}(t)|\rho(0) \oplus \rho(0) \oplus \rho(0) \oplus \rho(0)\rangle = |\rho(t) \oplus d_1 \oplus d_2 \oplus d_3\rangle, \quad (8)$$

where $\oplus$ indicates the direct sum of vectors and where

$$\hat{U} = \begin{pmatrix} \hat{S}_m & 0 & 0 & 0 \\ 0 & -\hat{S}_p & 0 & 0 \\ 0 & 0 & -\hat{A}_m & 0 \\ 0 & 0 & 0 & \hat{A}_p \end{pmatrix}. \quad (9)$$

$\hat{R}$ is a rotation operator to perform linear combinations of the propagated density matrices as described in Ref. [54], and the vectors d_1, d_2, d_3 are other linear combinations of propagated vectors on the dilated Hilbert space but are, in general, not equal to the propagated density matrix $\rho(t)$. Other approaches for the linear combination of unitaries are also known [72,73].

The operators on the diagonal of $\hat{U}$ are as follows:

$$\hat{S}_m = -\hat{S}_p^\dagger = ie^{-i\epsilon\hat{S}}$$
$$\hat{A}_m = \hat{A}_p^\dagger = e^{-\epsilon\hat{A}}. \tag{10}$$

Each of these operators is representable by a $k \times k$ matrix with k being the length of the vectorized density matrix. In this fashion, any nonunitary operator can be implemented on a quantum device as a sum of unitary operators. The block-diagonal gate $\hat{U}$ can be implemented as uniform controlled rotations or a multiplexed gate [74–78]. Here we implement $\hat{U}$ using QISKIT's gate transpiler for general gates [79].

The UME propagates the vectorized density matrix with a nonunitary propagator. In contrast to the operator-sum approach using Kraus operators, the propagation of the UME results in a propagated vectorized density matrix. Hence, upon observation of the state on a quantum simulator or device, the measured quantity yields the outer product of the propagated density-matrix vector with itself, i.e., $|\rho(t)\rangle\langle\rho(t)|$. The implementation of the nonunitary operator is the same in both cases, but in the case of the UME, the Z-basis measurement yields the square of the populations. The measurement of observables can be achieved by either density-matrix reconstruction or the Hadamard test circuit [57].

The dilation required by the decomposition presented here requires quantum circuits which are too deep to use on currently available quantum devices; therefore, we utilize QISKIT's QASM simulator for all emulation results. For all simulations, the expansion parameter is fixed, $\epsilon = 0.1$, and we simulate 2^{19} shots to obtain quality statistics. In the systems studied here, $\epsilon = 0.1$ was found to give near-exact results using the Taylor expansion above. The accuracy of the quantum algorithm is sensitive to the magnitude of ϵ due to noise on quantum devices; however, the convergence of Eq. (7) is second order in ϵ, and techniques, such as Richardson's extrapolation can be used on NISQ devices to accelerate the convergence [54,71].

Due to the vectorized density matrix, the qubit scaling in this implementation is less favorable than a wave-function-based propagation. If the density matrix is size $m \times m$, then the vectorized density matrix is length m^2, and the operator U is size $4m^2 \times 4m^2$. The dilation presented in Eq. (8) bounds the number of qubits n with the relation $n \geqslant \log_2 4m^2$. For example, a two-level system requires four qubits, and a four-level system requires six qubits in the present algorithm. This scaling can be reduced to $n \geqslant \log_2 2m^2$ by exploiting the block-diagonal structure of U as presented in Ref. [54]. In that case several circuits are required to reconstruct the complete dynamics of a given operator.

The major cost of the algorithm comes from the implementation of the operator $\hat{U}$ in Eq. (8). Here we use QISKIT's operator decomposer for general gates which assumes no structure in the operator; however, the form of $\hat{U}$ is a product of uniform controlled rotations, or a multiplexor. A general n-qubit unitary can be implemented with $O(n^2 4^n)$ one- and two-qubit gates, where $n \geqslant \log_2 4m^2$ [80]. The unitary U has a block-diagonal structure and can be implemented as controlled rotations [74–78]. Uniform controlled rotations are typically nontrivial to implement in quantum circuits; strategies and techniques to efficiently implement these controlled gates would result in a circuit depth reduction in the algorithm presented here. We use the general circuit decomposition from QISKIT for ease of implementation; a device-based experiment would require a more careful preparation of the desired circuits.

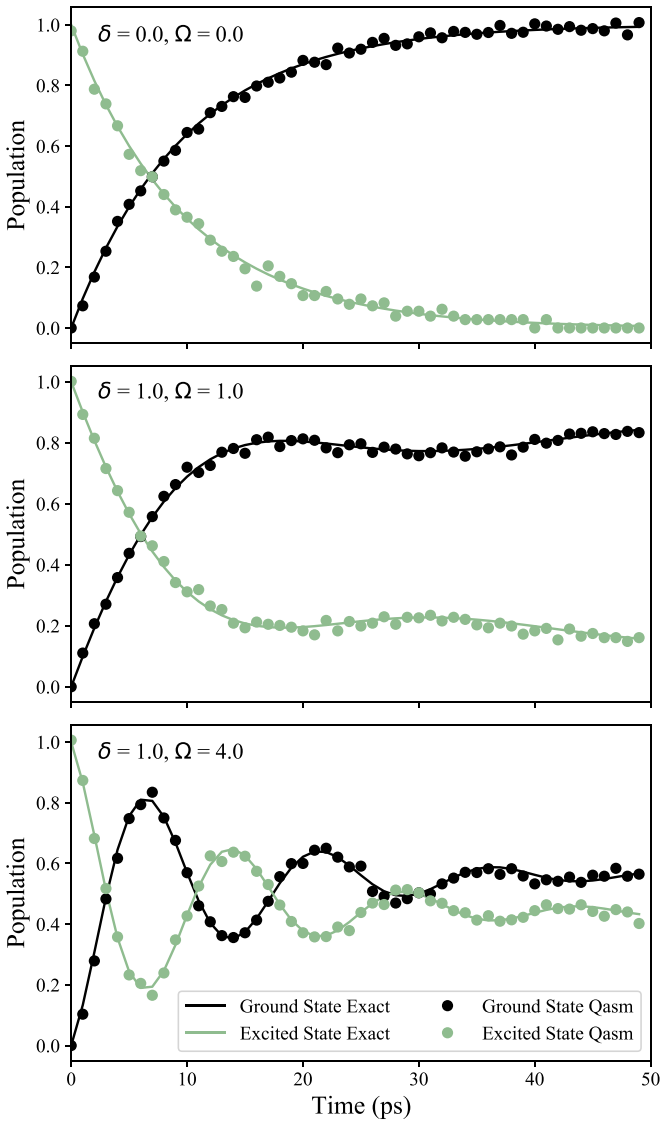

FIG. 1. Ground (black) and excited (green) state populations of a two-level system with an amplitude damping channel using QASM with 2^{19} shots, $\epsilon = 0.1$, $\gamma = 1.0$ with various values for δ and Ω.

III. RESULTS

We apply this unitary decomposition of operators to the quantum simulation of two models of open-system dynamics propagated according to the unraveled master equation. First, we study the dynamics of a two-level system with an amplitude damping channel under the Hamiltonian,

$$\hat{H} = -\frac{\delta}{2}\hat{\sigma}_z - \frac{\Omega}{2}\hat{\sigma}_x, \tag{11}$$

with a damping Lindbladian $\hat{C} = \sqrt{\gamma}\hat{\sigma}_-$. Figure 1 shows the dynamics in several different parameter regimes. We fix the amplitude damping $\gamma = 1.0$ for all simulations, whereas varying the detuning parameter δ and the Rabi frequency Ω to achieve qualitatively different dynamics. The exact solution is shown with the solid lines, and the simulation of the dynamics using QISKIT's QUASM simulator is shown by the dots. The quantum simulation obtains excellent agreement with the exact solution for the populations in all parameter regimes.

We also apply the present method to the transverse-field Ising model (TFIM) with two sites, resulting in a four-level system. The TFIM Hamiltonian has parameters describing the nearest-neighbor coupling strength (J) as well as the transverse magnetic-field strength (h),

$$\hat{H} = J \sum_i \hat{\sigma}_z^i \hat{\sigma}_z^{i+1} - h \sum_i \hat{\sigma}_x^i. \tag{12}$$

A single damping Lindbladian is also associated with each site $\hat{C} = \sqrt{\gamma}\hat{\sigma}_-^i$. The four-level TFIM has a twoold degenerate excited state as well as a nondegenerate excited state. We set the initial state to be the nondegenerate excited state, and for all simulations, we fix $J = 1$ and study the dynamics whereas differing h and γ. Inserting the Hamiltonians and Lindbladians into Eq. (3) generates the operators to perform the propagation.

Figure 2 shows the different dynamics under a range of magnetic-field strengths with the exact solution (solid lines), and results from the QASM simulator (markers). We omit one of the degenerate excited states for clarity, and we fix $J = 1.0$, $\gamma = 0.1$, $\epsilon = 1.0$, and utilize 2^{19} shots in the QASM simulator. With no magnetic field, there are no oscillations in the populations. As the field strength increases, the frequency of the oscillations also increases; however, the resulting steady state is not sensitive to the field strength. The QASM simulation results are in excellent agreement with the exact solution in all regimes of the magnetic-field parameter.

To further test the robustness of the algorithm, we also vary the damping parameter γ in the model. Figure 3 shows the population dynamics of the ground state in increasing damping regimes with fixed $J = h = 1.0$ and $\epsilon = 0.1$ using 2^{19} shots for the QASM simulator. The simulation (markers) obtain excellent agreement with the exact results (solid lines) in all regimes. As expected, as the damping parameter increases, the oscillations in the population are more quickly damped. In contrast to varying the magnetic-field strength, the resulting steady-state population is different for each choice of damping parameter.

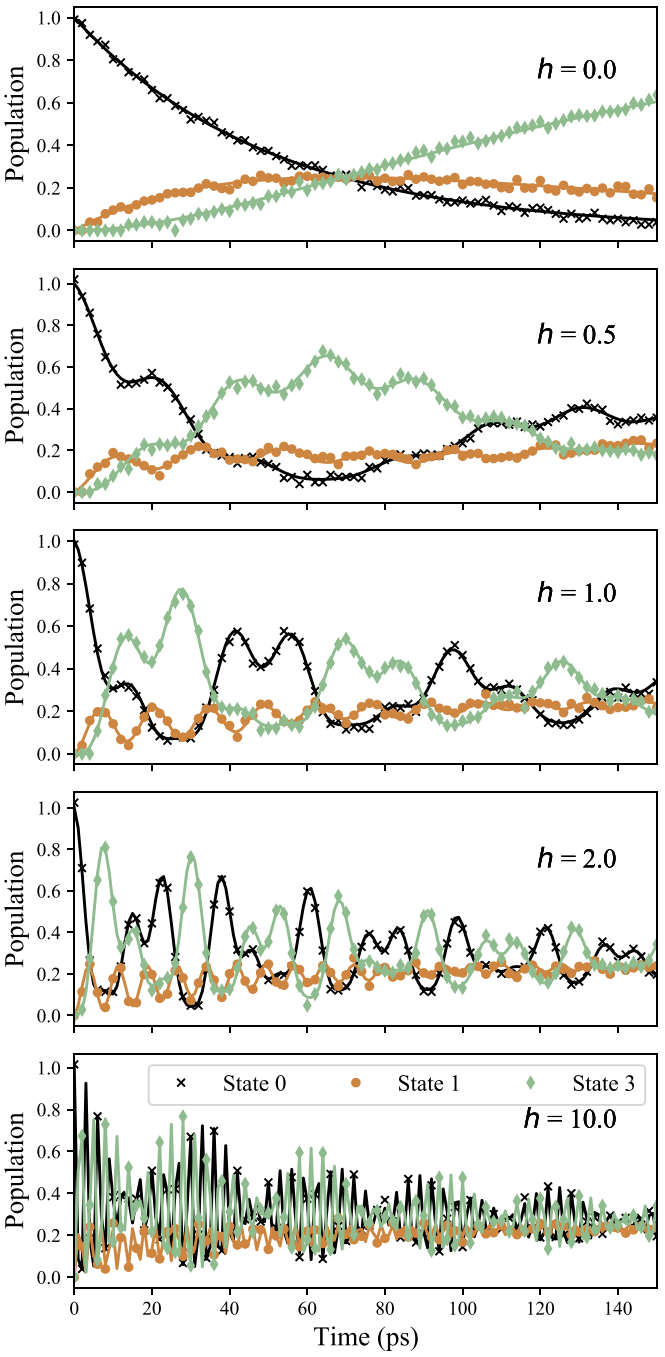

FIG. 2. Exact and simulated dynamics for the TFIM using various values of h, $\gamma = 0.1$, $J = 1.0$, and $\epsilon = 0.1$. The exact results are the solid lines, whereas the simulated results are denoted by the markers. We only include one copy of the degenerate excited states, states 1 and 2.

IV. CONCLUSIONS AND OUTLOOK

Here we presented a general unitary decomposition of operators to implement the nonunitary evolution of an open quantum system by the Lindblad equation in a quantum simulation. We demonstrated the robustness of the algorithm by investigating the parameter spaces of two-level and four-level model systems. The results of the simulator are highly accurate in all regimes of the parameter spaces studied, and the algorithm can be immediately implemented for other open quantum-system problems. The algorithm is completely general and can be used to implement any operator of interest in the framework of current quantum architecture.

Our current algorithm extends much of the recent work on modeling and predicting open quantum system evolution on quantum devices. The intersection of open quantum system dynamics with quantum computation shows much promise, both due to the potential exponential savings in the cost of the initial wave function or density matrix and due to the

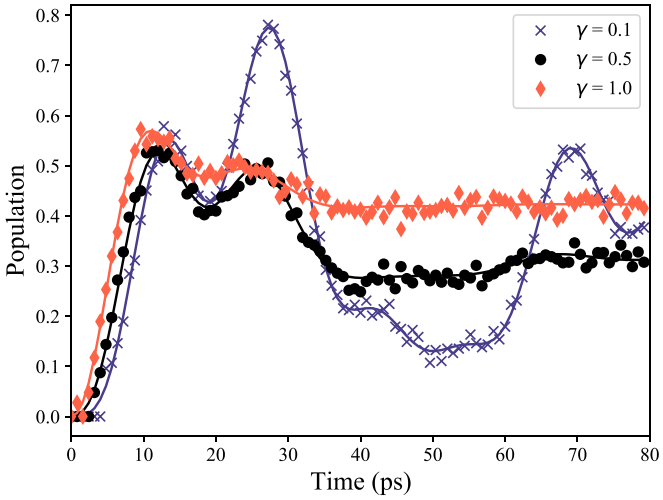

FIG. 3. QASM simulation of the TFIM ground state with 2^{19} shots using various γ's, $\epsilon = 0.1$, and $J = h = 1.0$. The exact classical solutions are the solid lines, whereas the QASM simulation results are denoted with the markers.

natural openness of the quantum hardware itself. Other studies have characterized the noise in the quantum hardware [51] and utilized it as a resource for the dynamics of an open quantum system [81]. Combining these novel algorithms for simulating open quantum systems whereas using the device noise as a resource for the dynamics offers a potential physical advantage to using quantum hardware for these types of processes.

The decomposition presented here dilates the nonunitary operator of interest and implements this operator in the form of controlled rotations. The multiqubit controlled gates can result in relatively deep circuits, which may lead to significant errors in its application on current NISQ devices. Nonetheless, as more efficient implementations of multiqubit uniform controlled rotations become available, this decomposition approach will become an increasingly practical means to model dynamic processes of open quantum systems. Furthermore, because the decomposition is completely general, it can be used to implement nonunitary processes in unitary-gate-based quantum computing.

Many investigations into the nonunitary time evolution of open quantum systems have relied on explicit mathematical dilation. Whereas this has been both effective and efficient, it requires the use of Kraus operators and, therefore, limits the applications to dynamics that can be written explicitly in the operator sum form. The strength of our algorithm is that it has no constraints on the operators used; lifting the constraint of requiring contraction mappings allows our method to work with the master equation directly. This drastically broadens the scope of applications of this algorithm as often the differential master equation is parametrized in a more physically meaningful way. Moreover whereas our current algorithm utilizes the unraveled Lindblad equation which is valid in the Markovian regime, we could use the algorithm to capture non-Markovian dynamics through use of the ensemble of Lindblad's trajectories method [10], which was previously applied in the explicit dilation framework. This algorithm has broad and far-reaching applications in quantum chemistry and quantum optics because it makes no explicit assumptions about the form of the propagators or nature of the dynamical regimes of interest.

ACKNOWLEDGMENTS

This work was supported by the NSF RAISE-QAC-QSA, Grant No. DMR 2037783 and the Department of Energy, Office of Basic Energy Sciences Grant No. DE-SC0019215. D. A. M. also acknowledges NSF EAGER Grant No. CHE-2035876 and NSF Grant No. CHE-1565638. We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM or the IBM Quantum team.

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