Doubling the order of approximation via the randomized product formula

Chien-Hung Cho,[1,2,*] Dominic W. Berry,[3,†] and Min-Hsiu Hsieh[2,‡]
[1]*Department of Physics, National Taiwan University, Taipei 10617, Taiwan*
[2]*Hon Hai (Foxconn) Quantum Computing Research Center, Taipei 114699, Taiwan*
[3]*School of Mathematical and Physical Sciences, Macquarie University, Sydney, NSW 2109, Australia*

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Hamiltonian simulation is a major application of quantum computing, for example, enabling prediction of the properties of molecules. Prior work has used product formulas with randomization to improve performance, but has only yielded modest improvements over the excellent performance provided by deterministic high-order product formulas. In this work, we provide a randomized scheme that greatly increases the order of product formulas, thereby providing a large advantage over the best-performing deterministic schemes. Our scheme is based on applying randomly chosen corrections to a high-order symmetric product formula. If the original product formula is of order $2k$ (so the error is of order $2k+1$), then the corrected formula is of order $4k+1$, corresponding to a doubling of the order of the error. In practice, applying the corrections in a quantum algorithm requires some structure to the Hamiltonian, for example, the Pauli strings as are commonly used in the simulation of quantum chemistry.

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I. INTRODUCTION

Simulating quantum systems is one of the critical applications for quantum computation, which was first proposed by Feynman [1]. When the size of the system increases, the number of parameters for describing the system grows exponentially, which leads to the difficulty of simulating such quantum systems on classical computers [2]. Therefore, one could utilize the power of quantum computers to further understand the behavior of these complex quantum systems in a range of fields, for instance, quantum chemistry [3–7], condensed matter physics [8], and high-energy physics [9].

Given the Hamiltonian $H=\sum_{j=1}^{L}H_j$, the main task of quantum simulation is to construct the approximated form of the unitary, $V:=\exp(-it\sum_{j=1}^{L}H_j)$, denoted as U, with elementary gates, and how to achieve this accurately and efficiently are two pivotal issues. To accurately approximate V, it is required that the error between U and V is, at most, ϵ, while the usage of the number of qubits or elementary gates for constructing the unitary U should be as small as possible. Often, the error is described by the criterion $\|U-V\|\leqslant\epsilon$ in terms of the spectral norm, though for randomized formulas the diamond norm of the channel is used.

Product formulas are one of the widely used quantum simulation methods due to their simplicity for near-term devices [10,11] and have gained more attention in recent years. In 1996, Lloyd proposed the first-order approximation to simulate the local system with the Hamiltonian [12], $H=\sum_{j=1}^{L}H_j$, by splitting time interval t into r steps,

$$e^{-iHt}\approx(e^{-iH_1t/r}e^{-iH_2t/r}\cdots e^{-iH_Lt/r})^r. \tag{1}$$

We choose a sufficiently large total number of steps, r, to ensure that the overall simulation error is, at most, ϵ. To have the higher-order approximation, Suzuki developed a method to systematically generate a product formula with $(2k)$th-order approximation, denoted as S_{2k} [13]. If we split the simulation time t into r steps, then for each step, S_{2k} approximates the target unitary V in the sense that

$$\|V(t/r)-S_{2k}(t/r)\|=O[(t/r)^{2k+1}]. \tag{2}$$

While there are several advanced techniques that have better asymptotic performance than product formulas [14–20], product formulas still perform well [21] when combined with information on the Hamiltonian structure [22].

Recently, several modifications based on randomization for product formulas have been proposed. Zhang showed that product formulas with some randomized strategies are easier to implement, but have the same efficiency compared to some deterministic product formulas [23]. Childs *et al.* proved the usefulness of randomly permuting over the summands of the Hamiltonian in the Trotter-Suzuki formula [24], which can have better gate complexity than deterministic Trotter-Suzuki formulas. However, both the randomized Trotter from Childs *et al.* and deterministic Trotter-Suzuki formulas suffer from scaling problems when the number of summands in the Hamiltonian grows to a large number. Consequently, Campbell proposed the qDRIFT protocol and improved the dependence of the number of summands in the Hamiltonian in gate complexity [25,26]. Due to quadratic dependence on variable time t, qDRIFT performs better for a short time, but gets worse after a specific critical time. Combining both

*f06222035@ntu.edu.tw
†dominic.berry@mq.edu.au
‡min-hsiu.hsieh@foxconn.com

TABLE I. The comparison of the complexity of various methods in terms of the number of exponentials.

Method	No. exponentials
$(2k)$th-order Trotter-Suzuki method	$O[tL^2(tL/\epsilon)^{\frac{1}{2k}}]$
$(2k)$th-order randomized product formula [24]	$\max\{O[tL^2(tL/\epsilon)^{\frac{1}{4k+1}}],\ O[tL^2(t/\epsilon)^{\frac{1}{2k}}]\}$
$(4k+1)$th-order modified randomized formula	$O[tL^2(tL/\epsilon)^{\frac{1}{4k+1}}]$

advantages of qDRIFT and first-order randomized Trotter, Ouyang *et al.* proposed a randomized simulation algorithm, called SPARSTO, to simulate the Hamiltonian through stochastical sparsification [27].

Applying randomization to further improve product formulas is, therefore, an important research topic for quantum simulation. We build on existing product formulas and exploit the properties of the randomized unitary channel to develop formulas with higher accuracy. In particular, we are motivated by this question: *Is it possible to correct the higher-order error by using randomization over the product formula?*

Overview of main results

The answer to the above question is affirmative. In this paper, we propose a procedure to systematically construct the randomized formula with higher-order approximation, and we refer to all such formulas as the *modified randomized formula*. Our method can be applied in general, but to simulate evolution under correction terms, it is most convenient if the Hamiltonian is a sum of Pauli strings. Starting from the $(2k)$th-order approximation, our procedure allows us to increase the error order of the modified randomized formula by averaging over a correction term. This generates the modified randomized formula with $(4k+1)$th-order approximation. As usual in this terminology, an order $2k$ approximation has error order $2k+1$, so the order of the error is being doubled from $2k+1$ to $4k+2$.

We analyze the performance of our methods using the mixing lemma [28]. First, we calculate the distance between each sampled unitary and the target unitary. Next, we calculate the distance between the average of the sampled unitaries and the target unitary. With the aid of the mixing lemma, when simulating the Hamiltonian $H=\sum_{j=1}^{L}H_j$ for time t, we can bound the diamond-norm distance between the randomized unitary channel proposed in this paper and the target quantum channel. For time t broken into r intervals, this gives the diamond-norm distance $O[(tL)^{4k+2}/r^{4k+1}]$ for the $(4k+1)$th-order approximation. If the diamond-norm distance may be no larger than ϵ, then the number of exponentials needed is $O[tL^2(tL/\epsilon)^{\frac{1}{4k+1}}]$. The overall gate complexity of these algorithms is proportional to the number of exponentials.

In our method, the complexity of the modified randomized formula performs better than the deterministic Trotter-Suzuki formula. It also outperforms the randomized product formula proposed by Childs *et al.* when t/ϵ is large. We list the complexity of different methods in Table I. The $(4k+1)$th-order approximation provides improvements over the deterministic $(2k)$th-order Trotter-Suzuki formula with respect to all parameters of interest. As a comparison, if the term $O[tL^2(tL/\epsilon)^{\frac{1}{4k+1}}]$ dominates in the complexity of the $(2k)$th-order randomized product formula, our $(4k+1)$th-order approximation has the same complexity in this case. When $L=o[(t/\epsilon)^{1+1/2k}]$, the term $O[tL^2(t/\epsilon)^{\frac{1}{2k}}]$ dominates in the complexity of the $(2k)$th-order randomized product formula, and our $(4k+1)$th-order approximation is advantageous.

The paper is structured as follows. We provide preliminaries in Sec. II, including basic concepts of norms, mixing lemma, and Trotter-Suzuki formula. Section III contains our main theoretic contribution and the recipe for constructing the modified randomized formula. The numerical comparison of various product formulas through the simulation of the Heisenberg system is presented in Sec. IV. The proof of our main result is provided in Appendix C.

II. PRELIMINARIES

In this section, we introduce some basic notations and properties of the norm, and those who are already familiar with these contents can directly skip this part.

A. Norms

Given the vector $\boldsymbol{\alpha}:=[\alpha_1,\alpha_2,\alpha_3,\ldots,\alpha_L]\in\mathbb{C}^L$, we define the ℓ_2 norm for the vector $\boldsymbol{\alpha}$ as

$$\|\boldsymbol{\alpha}\|_2:=\sqrt{\sum_{j=1}^{L}|\alpha_j|^2}. \tag{3}$$

If there is a matrix $A\in\mathbb{C}^{L\times L}$, the trace norm and the spectral norm are defined as

$$\|A\|_1:=\mathrm{Tr}(\sqrt{AA^\dagger}),\qquad \|A\|:=\max_{\boldsymbol{a}}\frac{\|A\boldsymbol{a}\|_2}{\|\boldsymbol{a}\|_2}. \tag{4}$$

Next, we define the norm for the superoperator. The diamond norm of the map $\mathcal{E}$ is defined as

$$\|\mathcal{E}\|_\diamond:=\max_{\rho:\|\rho\|_1\leqslant 1}\|(\mathcal{E}\otimes\mathbb{1})(\rho)\|_1, \tag{5}$$

where $\mathbb{1}$ acts on the same size of Hilbert space as $\mathcal{E}$. The submultiplicativity of the diamond norm is

$$\|AB\|_\diamond\leqslant\|A\|_\diamond\|B\|_\diamond, \tag{6}$$

and this implies $\|A^n\|_\diamond\leqslant\|A\|_\diamond^n$.

B. Trotter-Suzuki formula

To simulate the dynamics of a system with the Hamiltonian $H=\sum_{j=1}^{L}H_j$, many methods have been proposed to approximate the exponentiation,

$$V(\lambda):=\exp\left(\lambda\sum_{j=1}^{L}H_j\right), \tag{7}$$

where $\lambda \in \mathbb{C}$. For Hamiltonian simulation, $\lambda = -it$. The $(2k)$th-order Trotter-Suzuki formula is defined as [13]

$$S_2(\lambda) := \prod_{i=1}^{L} e^{\frac{\lambda}{2}H_i} \prod_{i=L}^{1} e^{\frac{\lambda}{2}H_i},$$

$$S_{2k}(\lambda) := S_{2k-2}(p_k\lambda)^2 S_{2k-2}[(1-4p_k)\lambda] S_{2k-2}(p_k)^2, \quad (8)$$

where $p_k := 1/(4-4^{1/(2k-1)})$, and for each S_{2k}, there are $N = 2\times 5^{k-1}(L-1)+1$ exponential terms in S_{2k}. We could define $\mathcal{S}_{2k}$ as the quantum channel corresponding to the unitary transformation S_{2k}. It is also possible to construct other symmetric product formulas [29]. Our method works for these general formulas, though we will discuss the costing for the Trotter-Suzuki formula to be specific.

C. Randomized product formula

The work of Childs *et al.* [24] demonstrates the efficacy of sampling the product formulas with random ordering of the Hamiltonian summands to improve the approximation of $\mathcal{V}(\lambda) : \rho \mapsto V(\lambda)\rho V(\lambda)^\dagger$, $\lambda \in \mathbb{C}$. For instance, considering the Hamiltonian $H = H_1 + H_2$, two product formulas with different ordering of the Hamiltonian summands are defined as follows:

$$S_1^{H_1H_2}(\lambda) := \exp(\lambda H_1)\exp(\lambda H_2),$$

$$S_1^{H_2H_1}(\lambda) := \exp(\lambda H_2)\exp(\lambda H_1).$$

By averaging these two product formulas, $V(\lambda)$ can be approximated to second order,

$$\left\| V(\lambda) - \frac{\left[S_1^{H_1H_2}(\lambda) + S_1^{H_2H_1}(\lambda)\right]}{2} \right\| \leqslant O[(\Lambda|\lambda|)^3], \quad (9)$$

where $\Lambda := \max\{\|H_1\|, \|H_2\|\}$. Practically, they achieve the approximation of $\mathcal{V}(\lambda)$ by uniformly and randomly sampling the operators $S_1^{H_1H_2}(\lambda)$ and $S_1^{H_2H_1}(\lambda)$ with the error bound in the diamond norm,

$$\left\| \mathcal{V}(\lambda) - \frac{\left[\mathcal{S}_1^{H_1H_2}(\lambda) + \mathcal{S}_1^{H_2H_1}(\lambda)\right]}{2} \right\|_\diamond \leqslant O[(\Lambda|\lambda|)^3], \quad (10)$$

where $\mathcal{S}_1^{H_1H_2}(\lambda)$ and $\mathcal{S}_1^{H_2H_1}(\lambda)$ denote the quantum channels for the operators $S_1^{H_1H_2}(\lambda)$ and $S_1^{H_2H_1}(\lambda)$, respectively. This diamond-norm error bound is analyzed using the mixing lemma [24], as summarized in the next section.

In general, this method can extend to higher-order product formulas $S_{2k}(\lambda)$. For the Hamiltonian with L summands, $H = \sum_{i=1}^{L} H_i$, randomly sampling the product formula with different orderings of the Hamiltonian summands gives the channel

$$\frac{1}{L!}\sum_{\sigma\in \mathrm{Sym}(L)} \mathcal{S}_{2k}^{\sigma}(\lambda), \quad (11)$$

which asymptotically improves the approximation of $\mathcal{V}(\lambda)$ [24]. Here, $\mathcal{S}_{2k}^{\sigma}(\lambda)$ is the quantum channel for the operator $S_{2k}^{\sigma}(\lambda)$, where $\sigma \in \mathrm{Sym}(L)$. $S_{2k}^{\sigma}(\lambda)$ is defined recursively as

$$S_2^{\sigma}(\lambda) := \prod_{i=1}^{L} e^{\frac{\lambda}{2}H_{\sigma(i)}} \prod_{i=L}^{1} e^{\frac{\lambda}{2}H_{\sigma(i)}}, \quad (12)$$

$$S_{2k}^{\sigma}(\lambda) := S_{2k-2}^{\sigma}(p_k\lambda)^2 S_{2k-2}^{\sigma}[(1-4p_k)\lambda] S_{2k-2}^{\sigma}(p_k)^2. \quad (13)$$

D. Mixing lemma

One can approximate the target channel by using the random unitary quantum channel. The following lemma shows that the diamond-norm distance between them can be bounded by considering two factors [28,30]: one is the distance between each sampled unitary and V, and the other one is the distance between the average of the unitary operators and V.

Lemma 1. (*Mixing lemma*). Let V be a target unitary, with a corresponding channel $\mathcal{V} : \rho \mapsto V\rho V^\dagger$. Let $a, b > 0$ and $\{U_1, U_2, U_3, \ldots, U_n\}$ be a set of unitary operators used to form a quantum channel $\mathcal{E} : \rho \mapsto \sum_{j=1}^{n} p_j U_j \rho U_j^\dagger$ such that

(1) $\|V - U_j\| \leqslant a$ for all $j \in \{1, 2, \ldots, n\}$,

(2) $\|V - \sum_{j=1}^{n} p_j U_j\| \leqslant b$ with some positive numbers p_j and $\sum_{j=1}^{n} p_j = 1$.

Then the error between the quantum channel $\mathcal{E}$ and $\mathcal{V}$ is bounded as $\|\mathcal{E} - \mathcal{V}\|_\diamond \leqslant a^2 + 2b$.

III. MAIN RESULTS

We first introduce the problem of interest in this paper and give the diamond-norm distance between the modified randomized quantum channel and the target channel. Next, we provide the recipe for constructing such a modified randomized quantum channel at the end of this section.

Problem 1. The Hamiltonian is in the form of $H = \sum_{j=1}^{L} H_j$. The problem is to present a recipe for generating the randomized product formula for a $(4k+1)$th-order approximation. In particular, we wish to construct such a modified randomized product formula with the higher-order approximation based on the order $2k$ Trotter-Suzuki formula.

Theorem 1. Consider the Hamiltonian $H = \sum_{j=1}^{L} H_j$, and the unitary operator $V = \exp(\lambda \sum_{j=1}^{L} H_j)$, which corresponds to the quantum channel $\mathcal{V} : \rho \mapsto V\rho V^\dagger$, where $\lambda = -it/r$. There exists a set of unitaries $\{\widetilde{U}_{h,l}\}$ and probabilities $\{p_{h,l}\}$ which define the random unitary quantum channel $\mathcal{E} : \rho \mapsto \sum_{h,l} p_{h,l}\widetilde{U}_{h,l}\rho\widetilde{U}_{h,l}^\dagger$ such that the error between $\mathcal{E}$ and $\mathcal{V}$ is bounded as

$$\|\mathcal{V}(\lambda) - \mathcal{E}(\lambda)\|_\diamond \leqslant a^2 + 2b, \quad a = 2A, \quad (14)$$

$$b = 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{4k+2}}{(4k+2)!}\exp[(5^{k-1}+1/2)|\lambda|L\Lambda] + \frac{A^2}{2}\exp(A) + \frac{3A^2}{4} + \frac{A^3}{4}, \quad (15)$$

where

$$A \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!}\exp[(5^{k-1}+1/2)|\lambda|L\Lambda], \quad (16)$$

and $\Lambda := \max_j\{\|H_j\|\}$.

This theorem is obtained by using a $(2k)$th-order Trotter-Suzuki product formula, with the unitaries $\widetilde{U}_{h,l}$ corresponding to two steps under the Trotter-Suzuki formula with a random correction in between. The part here that is specific to the Trotter-Suzuki formula is 5^{k-1}. One could also use other symmetric product formulas of order $2k$ that would yield a

different factor here. The proof of Theorem 1 is provided in Appendix C.

Theorem 1 bounds the error between the quantum channel $\mathcal{E}$ and $\mathcal{V}$, which can be used to give an expression for the asymptotic error. Taking Λ to be a constant, we set $k \in \mathbb{N}$, and $r \geqslant (5^{k-1}+1/2)tL\Lambda$. We then have the asymptotic error for the modified randomized formula,

$$\|\mathcal{V}(-it) - \mathcal{E}^r(-it/r)\|_\diamond \leqslant O\left[\frac{(tL)^{4k+2}}{r^{4k+1}}\right]. \tag{17}$$

To ensure that the simulation error is, at most, ϵ, it suffices to use the number of segments,

$$r^m_{4k+1} = O\left[tL\left(\frac{tL}{\epsilon}\right)^{\frac{1}{4k+1}}\right]. \tag{18}$$

Multiplying by L gives the order of the number of exponentials for the simulation,

$$g^m_{4k+1} = O\left[tL^2\left(\frac{tL}{\epsilon}\right)^{\frac{1}{4k+1}}\right]. \tag{19}$$

In contrast, for the case of the Trotter-Suzuki formula, the diamond-norm distance between $\mathcal{S}_{2k}$ and $\mathcal{V}$ is [24]

$$\|\mathcal{V}(-it) - \mathcal{S}^r_{2k}(-it/r)\|_\diamond \leqslant O\left[\frac{(tL)^{2k+1}}{r^{2k}}\right]. \tag{20}$$

To guarantee that the error is, at most, ϵ, the number of segments, r^{ts}_{2k}, satisfies

$$r^{ts}_{2k} = O\left[tL\left(\frac{tL}{\epsilon}\right)^{\frac{1}{2k}}\right], \tag{21}$$

and this gives the number of exponentials,

$$g^{ts}_{2k} = O\left[tL^2\left(\frac{tL}{\epsilon}\right)^{\frac{1}{2k}}\right]. \tag{22}$$

When comparing to Eq. (19), one can see that our method provides improvement to all parameters of interest. As a comparison, for the randomized formula proposed by Childs *et al.* [24], its number of exponentials, g^{rand}_{2k}, is

$$g^{\text{rand}}_{2k} = \max\left\{O\left[tL^2\left(\frac{tL}{\epsilon}\right)^{\frac{1}{4k+1}}\right], \quad O\left[tL^2\left(\frac{t}{\epsilon}\right)^{\frac{1}{2k}}\right]\right\}. \tag{23}$$

When the first term in Eq. (23) dominates, our method has the same performance as their randomized formula. When $L = o[(t/\epsilon)^{1+1/2k}]$, the second term in Eq. (23) dominates and our modified randomized formula is advantageous. In practice, we further decompose each exponential into universal elementary gates in the quantum computer. This results in, at most, a constant multiplicative factor for the number of elementary gates. The exact number of gates depends on the choice of the elementary gate for the type of hardware, which is beyond the scope of our discussion.

A. Recipe for the construction of the formula

We construct the quantum channel

$$\mathcal{E}{:}\rho \mapsto \sum_{h,l} p_{h,l}\widetilde{U}_{h,l}\rho\widetilde{U}^\dagger_{h,l}, \tag{24}$$

with the well-designed unitary $\{\widetilde{U}_{h,l}\}$ and corresponding probabilities $\{p_{h,l}\}$ to approximate $\mathcal{V}$. In our scheme, specifying a number $k \in \mathbb{N}$, we could construct each unitary in $\{\widetilde{U}_{h,l}\}$ based on any symmetric $(2k)$th-order formula, but, to be specific, we restrict our discussion to Suzuki's recursive construction of product formulas, S_{2k}. According to the mixing lemma, the accuracy of this approximation is determined by two factors: the distance between V and each sampled unitary, and the distance between V and the average of unitaries.

For the higher-order randomized product formulas from [24], the first factor contributes the $O[(|\lambda|\Lambda)^{4k+2}]$ error, while the contribution from the second factor, an average of unitary, is dominant with the $O[(|\lambda|\Lambda)^{2k+1}]$ error. Therefore, we aim to design $\{\widetilde{U}_{h,l}\}$ and $\{p_{h,l}\}$ such that the average of unitaries, denoted as $S^{\text{avg}}_{4k+1}(\lambda)$, satisfies

$$\left\|V(\lambda) - S^{\text{avg}}_{4k+1}(\lambda)\right\| = O[(|\lambda|\Lambda)^{4k+2}], \tag{25}$$

where $S^{\text{avg}}_{4k+1} := \sum_{h,l} p_{h,l}\widetilde{U}_{h,l}$. According to the mixing lemma, that will then enable the same order of approximation in the channel $\mathcal{E}$.

Our principle is to use two applications of $S_{2k}(\lambda/2)$ (half the time) with a well-designed unitary correction, denoted as $U^{(l)}_h$, in between to construct $\widetilde{U}_{h,l}$ as

$$\widetilde{U}_{h,l} := S_{2k}(\lambda/2)U^{(l)}_h S_{2k}(\lambda/2). \tag{26}$$

This sandwich structure ensures that the modified product formula is still symmetric, allowing us to correct the error up to order $(4k+1)$ by choosing the unitary correction according to the probabilities $\{p_{h,l}\}$. To achieve this, we will choose a set of unitaries, $\{U^{(l)}_h\}$, and the corresponding probabilities $\{p_{h,l}\}$ such that

$$\sum_{h,l} p_{h,l}U^{(l)}_h = \mathbb{1} - V^\dagger D - DV^\dagger + O(\lambda^{4k+2}), \tag{27}$$

where

$$D(\lambda/2) := S_{2k}(\lambda/2) - V(\lambda/2). \tag{28}$$

Here, all quantities with the argument omitted are for $\lambda/2$. It is found that

$$\begin{aligned}
&S_{2k}(\lambda/2)(\mathbb{1} - V^\dagger D - DV^\dagger)S_{2k}(\lambda/2)\\
&\quad= S_{2k}(\lambda/2)(\mathbb{1} - V^\dagger D)(\mathbb{1} - DV^\dagger)S_{2k}(\lambda/2) + O(\lambda^{4k+2})\\
&\quad= S_{2k}(\lambda/2)(\mathbb{1} + V^\dagger D)^{-1}(\mathbb{1} + DV^\dagger)^{-1}S_{2k}(\lambda/2)\\
&\qquad+ O(\lambda^{4k+2})\\
&\quad= S_{2k}(\lambda/2)(V^\dagger S_{2k})^{-1}(S_{2k}V^\dagger)^{-1}S_{2k}(\lambda/2) + O(\lambda^{4k+2})\\
&\quad= V(\lambda) + O(\lambda^{4k+2}).
\end{aligned} \tag{29}$$

This implies that the choice of randomized operators will satisfy Eq. (25) as required.

What remains to be shown is that it is possible to choose the operators such that Eq. (27) is satisfied. The general principle is that the error in $S_{2k}(\lambda/2)$ is of order $2k+1$, so $V^\dagger D + DV^\dagger$ can be expanded as a sum of terms of order $2k+1$ and higher. We can, therefore, take $\{U^{(l)}_h\}$ to be exponentials of the negatives of these terms. The nonlinearity in the exponentials can be ignored because it is $O(\lambda^{4k+2})$.

More explicitly, we can write

$$V^\dagger D + DV^\dagger = \sum_{l\in\gamma}\sum_{j=1}^{L_l} \frac{\lambda^l}{2^l}\beta_j^{(l)} H_j^{(l)} + O(\lambda^{4k+2}), \tag{30}$$

where γ is a set of orders used for the corrections, there are L_l elements at the lth order in λ, and we denote the jth terms as $\beta_j^{(l)} H_j^{(l)}$, for $\beta_j^{(l)} \in \mathbb{R}$. We will show that

(1) the even orders up to $4k$ cancel, and

(2) the operators $H_j^{(l)}$ are Hermitian.

That implies that the exponentials of the terms in the sum will yield unitary operators.

To show the first property, we define time reversibility and show a related result on the orders.

Definition 1 (*Time reversibility* [29]). Let $W(\lambda)$ be a symmetric product composition of several operators with the properties

$$W(\lambda)W(-\lambda) = W(-\lambda)W(\lambda) = \mathbb{1}, \tag{31}$$

for $\lambda \in \mathbb{C}$. Then we say the operator $W(\lambda)$ has time reversibility.

Lemma 2. Define $V(\lambda)$ as in Eq. (7) and $S_{2k}(\lambda)$ as in Eq. (8). The time-reversible properties of the symmetric operator, $[V^\dagger(\lambda/2)S_{2k}(\lambda/2)]^{-1}[S_{2k}(\lambda/2)V^\dagger(\lambda/2)]^{-1}$, result in the simultaneous vanishing of terms at even orders in $\{2k+2, 2k+4, \ldots, 4k\}$.

We provide the proof in Appendix A. Because $(V^\dagger S_{2k})^{-1}(S_{2k}V^\dagger)^{-1}$ is equal to $\mathbb{1} - V^\dagger D - DV^\dagger$ up to a correction of an order $(4k+1)$ according to Eq. (29), the same result holds for orders up to $(4k+1)$ in Eq. (30). Therefore, Lemma 2 implies that $\gamma = \{2k+1, 2k+3, \ldots, 4k+1\}$. This demonstrates that the first required property holds.

The second property, that $H_j^{(l)}$ are Hermitian, can be shown as follows. As described in the proof of Lemma 2, we can express $(V^\dagger S_{2k})^{-1}(S_{2k}V^\dagger)^{-1}$ as

$$\begin{aligned}&(V^\dagger S_{2k})^{-1}(S_{2k}V^\dagger)^{-1}\\ &\quad= \exp(\lambda^{2k+1}\mathcal{H}_{2k+1} + \lambda^{2k+3}\mathcal{H}_{2k+3} + \cdots),\end{aligned} \tag{32}$$

where $\mathcal{H}_l$ are linear combinations of products of l individual Hamiltonians from $\{H_j\}_{j=1}^L$. Because the exponential must be unitary, $\mathcal{H}_l$ must be Hermitian. Now, we write these operators as

$$\mathcal{H}_l = \sum_{j=1}^{L_l} \frac{\beta_j^{(l)}}{2^l} H_j^{(l)}, \tag{33}$$

for $l \in \gamma$. It is always possible to choose $H_j^{(l)}$ to be Hermitian. This is because if the Hermitian operator $\mathcal{H}_l$ was written as a sum with non-Hermitian $H_j'^{(l)}$, it could be written as exactly the same sum with all $H_j'^{(l)}$ replaced with $H_j'^{(l)\dagger}$. Averaging these two sums then gives the sum in Eq. (33) with $H_j^{(l)} = (H_j'^{(l)} + H_j'^{(l)\dagger})/2$, which is Hermitian as required.

To achieve the approximation in Eq. (27), we therefore aim to choose $\{p_{h,l}\}$ and $\{U_h^{(l)}\}$ such that

$$\sum_{h,l} p_{h,l} U_h^{(l)} = \mathbb{1} - \sum_{l\in\gamma}\sum_{j=1}^{L_l} \frac{\lambda^l}{2^l}\beta_j^{(l)} H_j^{(l)} + O(\lambda^{4k+2}), \tag{34}$$

with $\gamma = \{2k+1, 2k+3, \cdots, 4k+1\}$ and $\{H_j^{(l)}\}_{j=1}^{L_l}$ Hermitian operators obtained from the expansion of $V^\dagger D + DV^\dagger$. An appropriate choice is

$$U_h^{(l)} := \exp\left(\alpha_{h,l} H_h^{(l)}\right), \tag{35}$$

with the criterion for choosing $\{\alpha_{h,l}\}$ and $\{p_{h,l}\}$,

$$p_{h,l}\alpha_{h,l} = -\left(\frac{\lambda}{2}\right)^l \beta_h^{(l)}. \tag{36}$$

To show that the criterion works, we express the equation as

$$\begin{aligned}&\sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} U_h^{(l)}\\ &\quad= \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l}\left[\mathbb{1} + \alpha_{h,l} H_h^{(l)} + O(\lambda^{4k+2})\right]\\ &\quad= \left[\mathbb{1} - \sum_{l\in\gamma}\sum_{h=1}^{L_l}\left(\frac{\lambda}{2}\right)^l \beta_h^{(l)} H_h^{(l)}\right] + O(\lambda^{4k+2}).\end{aligned} \tag{37}$$

The criterion in Eq. (36) can be satisfied with multiple choices, but one that helps to reduce the error in the linear approximation of the exponential is

$$\alpha_{h,l} := -\frac{\operatorname{sgn}(\epsilon_{h,l})A}{\|H_h^{(l)}\|}, \tag{38}$$

$$p_{h,l} := \frac{|\epsilon_{h,l}|}{A}, \tag{39}$$

where

$$\epsilon_{h,l} := \left(\frac{\lambda}{2}\right)^l \beta_h^{(l)} \|H_h^{(l)}\|, \tag{40}$$

$$A := \sum_{l\in\gamma}\sum_{h=1}^{L_l} |\epsilon_{h,l}|. \tag{41}$$

Thus the procedure can be summarized as follows. First find the $H_h^{(l)}$ and $\beta_h^{(l)}$ from the expansion of $V^\dagger D + DV^\dagger$. Use these to choose $\alpha_{h,l}$ and $p_{h,l}$ according to the equations from Eq. (38) to Eq. (41). These are used to choose the random unitaries $U_h^{(l)}$ in Eq. (35) with probabilities $p_{h,l}$, to give the overall unitary,

$$\widetilde{U}_{h,l}(\lambda) := S_{2k}(\lambda/2)\, U_h^{(l)}\, S_{2k}(\lambda/2). \tag{42}$$

That is, the quantum channel can be expressed as

$$\mathcal{E} : \rho \mapsto \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l}\, \widetilde{U}_{h,l}\, \rho\, \widetilde{U}_{h,l}^\dagger. \tag{43}$$

Because our choice of random unitaries implies that Eq. (25) holds, the mixing lemma means that $\mathcal{E}$ is accurate to order $4k+1$ (with error order of $4k+2$).

This recipe also holds when S_{2k} is replaced with an average of order $2k$ symmetric product formulas. The reasoning to show that $S_{2k}(\lambda/2)(\mathbb{1} - V^\dagger D - DV^\dagger)S_{2k}(\lambda/2)$ is equal to $V(\lambda) + O(\lambda^{4k+2})$ holds unchanged. Then, the argument that $\mathbb{1} - V^\dagger D - DV^\dagger$ has only odd-order Hermitian terms up to order $4k+1$ holds for any single product formula in the average. If D is computed for the average over product formulas,

then the average will still be required to have only odd-order Hermitian terms. Some steps in our reasoning will not hold when using an average over symmetric product formulas, so we will not consider that case further.

Although this scheme holds for general Hamiltonians, implementing evolution under $H_j^{(l)}$ may be difficult. It can be implemented efficiently in the case for quantum chemistry. For the n-qubit chemistry system formulated in the second-quantized Hamiltonian, we can transfer it into a linear combination of Pauli strings,

$$H = \sum_{i=1}^{L} H_i = \sum_{i=1}^{L} h_i \bigotimes_{j=1}^{n} \sigma_i^j, \tag{44}$$

where $h_i \in \mathbb{R}$, and σ_i^j denotes an operator in $\{\mathbb{1}, X, Y, Z\}$ acting on the jth qubit. Here, X, Y, Z are Pauli operators. Since the correction terms $H_j^{(l)}$ consist of products involving l individual Hamiltonians from $\{h_i \bigotimes_{j=1}^{n} \sigma_i^j\}_{i=1}^{L}$, these correction terms could be either Hermitian or anti-Hermitian. From the reasoning above, Eq. (34) shows that the correction terms can be chosen to be Hermitian.

In addition, determining the full set of unitary corrections would be an issue for this modified formula. Classically determining the expansion of $V^\dagger D + DV^\dagger$ is easy for moderate order k and number of Hamiltonian terms, L. However, the number of correction terms increases exponentially with k, so it will be intractable for larger k and L. It may be possible to efficiently sample from these correction terms without needing to determine all terms. The development of an algorithm for sampling these correction terms classically remains an open question for future research.

B. A simple example of a modified randomized formula

Here, we demonstrate the construction of the modified randomized formula using a simple example with the system Hamiltonian $H = H_1 + H_2$. In this case, we construct the modified randomized formula based on $S_2(\lambda/2)$,

$$S_2(\lambda/2) = \exp(H_1\lambda/4)\exp(H_2\lambda/2)\exp(H_1\lambda/4). \tag{45}$$

Using the definition of $D(\lambda/2)$ in Eq. (28), we have the Taylor expansion of the operator up to fifth order in λ,

$$\begin{aligned}\mathbb{1} - V^\dagger D - DV^\dagger &= \mathbb{1} + \lambda^3(-H_1H_2H_1/48 + \cdots) + \lambda^5(H_1H_2H_2H_1H_2/384 \\ &+ H_2H_1H_2H_2H_1/384 + \cdots) + O(\lambda^6).\end{aligned} \tag{46}$$

Here all quantities with the argument omitted are for $\lambda/2$. For clarity, we present only a selection of terms from the expansion in Eq. (46). Due to the approximation in Eq. (30) and the result of Lemma 2, the terms at the fourth order vanish. In this case, we have $\gamma = \{3, 5\}$. With this information, we can construct the unitary $\{U_h^{(l)}\}$ and $\{p_{h,l}\}$ based on these expansion terms. For instance, considering the terms listed in Eq. (46), we construct the corresponding unitaries, denoted as $U_0^{(3)}$ and $U_0^{(5)}$,

$$\begin{aligned}U_0^{(3)} &= \exp(\alpha_{0,3}H_1H_2H_1), \\ U_0^{(5)} &= \exp[\alpha_{0,5}(H_1H_2H_2H_1H_2 + H_2H_1H_2H_2H_1)],\end{aligned} \tag{47}$$

with the condition

$$\begin{aligned}p_{0,3}\alpha_{0,3} &= -\frac{\lambda^3}{48}, \\ p_{0,5}\alpha_{0,5} &= \frac{\lambda^5}{384}.\end{aligned} \tag{48}$$

Once the full set of the expansion terms in Eq. (46) is known, we can design the entire set of terms in $\{p_{h,l}\}$ and $\{U_h^{(l)}\}$, satisfying the conditions from Eq. (38) to Eq. (41). Consequently, we can have a set of sampled unitaries, $\{S_2(\lambda/2)U_0^{(3)}S_2(\lambda/2), S_2(\lambda/2)U_0^{(5)}S_2(\lambda/2), \cdots\}$, with the corresponding probabilities $\{p_{0,3}, p_{0,5}, \cdots\}$. Based on these sampled unitaries and probabilities, the corresponding quantum channel, denoted as $\mathcal{E}(\rho)$, can approximate $V(\lambda)\rho V^\dagger(\lambda)$ up to fifth order in λ.

IV. COMPARISON AND NUMERICAL VALIDATION

We numerically compare the cost of simulating the dynamics of the Hamiltonian of the Heisenberg model with the size n,

$$H = \sum_{j=1}^{n}(X_jX_{j+1} + Y_jY_{j+1} + Z_jZ_{j+1} + Z_j),$$

where X_j, Y_j, and Z_j denote the corresponding Pauli operators acting on the jth site. This comparison involves three different types of simulation methods with $k = 2$ and $k = 3$: the deterministic Trotter-Suzuki method [13], the randomized formula [24], and our modified randomized formula. The fourth-order and sixth-order formulas exhibit the best performance when simulating the Heisenberg system with a size n ranging from ten to one hundred [21]. Our focus lies in understanding how the number of exponentials varies when the system size n and simulation time t change with the cases of the target error rate of $\epsilon = 10^{-3}$ and 10^{-6}. For the first comparison, we set $t = n$ and change the size n from 10 to 100, as considered in [24]. For the second comparison, we choose $n = 10$ and vary the time t from 0.1 to 10^6 to benchmark their asymptotic performance in long-time simulation.

Given the analytical error bound of the product formula, we perform a binary search to obtain the value of r, enabling one to evaluate the number of exponentials [21]. The error bounds used in this comparison for Trotter-Suzuki formulas and randomized formulas are based on the analytical bounds in Refs. [21] and [24], respectively.

In Figs. 1(a) and 1(b), we compare the performance of different formulas for simulating the system size n ranging from 10 to 100. We see that modified randomized formulas provide a significant improvement over Trotter-Suzuki formulas and randomized formulas. When simulating a system with a fixed target error $\epsilon = 10^{-3}$, we observe that the cost associated with the Trotter-Suzuki formula exceeds that of the randomized formula, while, in turn, the cost of the randomized formula is greater than that of the modified randomized formula. In addition, as the target error ϵ changes from 10^{-3} to 10^{-6}, the incremental cost increase associated with the modified randomized formula is smaller compared to the Trotter-Suzuki and randomized formula. For instance, when $n = 100$ and comparing $\epsilon = 10^{-3}$ to $\epsilon = 10^{-6}$, the difference

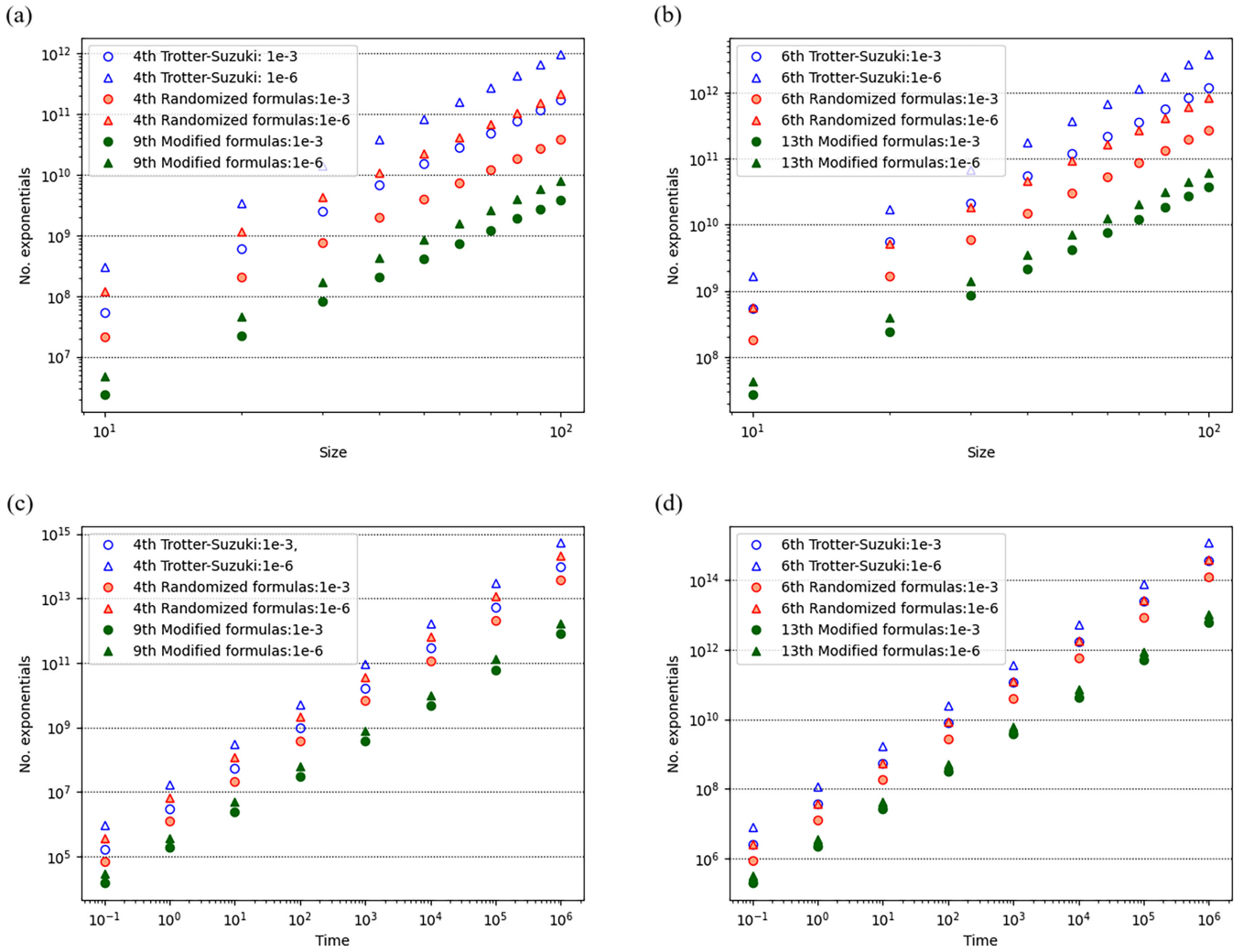

FIG. 1. (a), (b) Cost comparison for different system sizes with target errors of $\epsilon = 10^{-3}$ and $\epsilon = 10^{-6}$ using the formulas with (a) $k = 2$ and (b) $k = 3$. For each data point, we set $t = n$. (c),(d) Cost comparison over time with target errors of $\epsilon = 10^{-3}$ and $\epsilon = 10^{-6}$ using the formulas with (c) $k = 2$ and (d) $k = 3$ with $n = 10$.

in the number of exponentials for thirteenth-order modified randomized formulas is $1.206\,894 \times 10^{10}$. This difference is notably smaller than the corresponding values for sixth-order Trotter and randomized formulas, which are $1.211\,323 \times 10^{12}$ and $2.811\,499 \times 10^{11}$, respectively.

From Figs. 1(c) and 1(d), we can observe the advantage of the modified randomized formula over the Trotter-Suzuki and randomized formula in a long simulation time. When varying the simulation time, it is notable that the cost of the modified random formula exhibits a smaller rate of increase compared to the Trotter-Suzuki and randomized formula. Likewise, if ϵ is varied from 10^{-3} to 10^{-6}, the incremental cost associated with the modified random formula is lower than that of both the Trotter-Suzuki and randomized formula. In the given scenario, for example, at $t = 10^6$, when comparing the cases of $\epsilon = 10^{-3}$ to $\epsilon = 10^{-6}$, the difference in the number of exponentials for thirteenth-order modified randomized formulas amounts to $4.055\,405 \times 10^{12}$. This difference is notably smaller than the corresponding values for sixth-order Trotter and randomized formulas, which stand at $7.885\,884 \times 10^{14}$ and $2.588\,236 \times 10^{14}$, respectively.

V. DISCUSSION AND OUTLOOK

We propose a scheme for any symmetric $(2k)$th-order product formulas by randomizing over the formula with the correction unitary, which could double the order of error of the formulas. Our analysis provides the upper bound of the diamond-norm distance between the randomized channel proposed in this paper and the target unitary channel. Based on this analysis, we show that the gate complexity of our scheme is better than the deterministic $(2k)$th-order approximation, and performs better than the existing high-order randomized formula when $L = o[(t/\epsilon)^{1+1/2k}]$.

Doubling the error order of the formula achieved by our modified randomized scheme has profound implications for simulating quantum systems on quantum computers. Particularly advantageous for long-time simulations requiring high accuracy, our method significantly saves computing resources. This efficiency makes our randomized simulation techniques well suited for investigating complex many-body effects, such as localization. Additionally, our approach is highly applicable to fields with stringent accuracy requirements, such as

quantum chemistry, showcasing its versatility and potential impact across diverse domains.

In addition, it is worth investigating how our randomized scheme could combine with other Hamiltonian simulation schemes, such as the linear combination of unitary (LCU) [31], quantum signal processing (QSP), and qubitization, and we leave this as our future work.

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APPENDIX A: PROOF OF LEMMA 2

In the following part, we provide the proof of Lemma 2.

Proof. First, we show that ${S_{2k}}^\dagger V V {S_{2k}}^\dagger$ satisfies time reversibility. Because S_{2k} is a symmetric product formula, it satisfies time reversibility $S_{2k}(\lambda/2)S_{2k}(-\lambda/2) = \mathbb{1}$. Similarly, V satisfies time reversibility because it is the exact exponential. Thus, the symmetric operator ${S_{2k}}^\dagger V V {S_{2k}}^\dagger$ is also time reversible. Therefore, as a result of the lemma in [29], ${S_{2k}}^\dagger V V {S_{2k}}^\dagger$ corresponds to an exponential containing only *odd*-order terms in λ. Moreover, because S_{2k} is an $(2k)$th-order approximation of V, ${S_{2k}}^\dagger V V {S_{2k}}^\dagger$ is equal to the identity with the zero terms up to order $2k$ in λ. This leads to the first order that can have nonzero terms being $(2k+1)$. Then we can express ${S_{2k}}^\dagger V V {S_{2k}}^\dagger$ as in Eq. (32).

As a result, when we expand the exponential up to order $4k+1$, only odd-order terms are nonzero. The order $4k+2$ term in the expansion of the exponential may be nonzero because it comes from an order $2k+1$ term squared. We can see this by expanding Eq. (32),

$$\begin{aligned} {S_{2k}}^\dagger V V {S_{2k}}^\dagger = \mathbb{1} + \lambda^{2k+1}\mathcal{H}_{2k+1} + \lambda^{2k+3}\mathcal{H}_{2k+3} + \cdots \\ + \lambda^{4k+1}\mathcal{H}_{4k+1} + \tfrac{1}{2}(\lambda^{2k+1}\mathcal{H}_{2k+1})^2 + \cdots . \end{aligned} \tag{A1}$$

■

APPENDIX B: UPPER BOUND ON THE ERROR TERMS

In the following part, we bound the norm of the operators A and D defined in Eq. (41) and Eq. (28).

Lemma 3. Given the form of A and D as in Eq. (41) and Eq. (28), we have the upper bounds,

$$\begin{aligned} \|D\| \leqslant \frac{(5^{k-1}|\lambda|L\Lambda)^{2k+1}}{(2k+1)!}\exp(5^{k-1}|\lambda|L\Lambda) \\ + \frac{(|\lambda|L\Lambda/2)^{2k+1}}{(2k+1)!}\exp\left(|\lambda|L\Lambda/2\right) \end{aligned} \tag{B1}$$

and

$$A \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!}\exp[(5^{k-1}+1/2)|\lambda|L\Lambda]. \tag{B2}$$

Proof. Using the approach in [32], one can bound the size of terms in the expansion of the exponential at order s by replacing each operator with its norm. Replacing each operator in the exponentials of S_{2k} by their norms, you have (corresponding to Eq. (7) in [32])

$$[1 + |\lambda|\Lambda + (|\lambda|\Lambda)^2/2 + \ldots]^{2L5^{k-1}}. \tag{B3}$$

That gives the upper bound for the order-s terms in S_{2k} as

$$\frac{(2L5^{k-1}|\lambda|\Lambda)^s}{s!}. \tag{B4}$$

This expression is specific to the Trotter-Suzuki product formula. Similarly, the order s terms in the exact exponential of the Hamiltonian may be upper bounded as

$$\frac{(L|\lambda|\Lambda)^s}{s!}. \tag{B5}$$

By summing Eqs. (B4) and (B5), and replacing λ with $\lambda/2$, we can upper bound $\|D\|$ as

$$\begin{aligned} \|D\| &= \left\| \exp\left(\frac{\lambda}{2}\sum_{j=1}^{L} H_j\right) - S_{2k} \right\| \\ &\leqslant \sum_{s=2k+1}^{\infty}\frac{(2L5^{k-1}|\lambda|\Lambda/2)^s}{s!} + \sum_{s=2k+1}^{\infty}\frac{(L|\lambda|\Lambda/2)^s}{s!} \\ &\leqslant \frac{(5^{k-1}|\lambda|L\Lambda)^{2k+1}}{(2k+1)!}\exp(5^{k-1}|\lambda|L\Lambda) \\ &\quad + \frac{(|\lambda|L\Lambda/2)^{2k+1}}{(2k+1)!}\exp\left(|\lambda|L\Lambda/2\right). \end{aligned} \tag{B6}$$

From the definition in Eq. (41),

$$A := \sum_{l\in\gamma}\sum_{h=1}^{L_l}|\epsilon_{h,l}|, \tag{B7}$$

which corresponds to the sum of the magnitudes of the terms in $V^\dagger D + D V^\dagger$, where both quantities are for $\lambda/2$. To bound the norm of the higher-order terms in $V^\dagger D = V^\dagger S_{2k} - \mathbb{1}$, we can consider the corresponding higher-order terms in $V^\dagger S_{2k}$. Similarly, the higher-order terms in $DV^\dagger$ correspond to those in $S_{2k}V^\dagger$.

When multiplying S_{2k} by the inverse of the evolution, one can use the same approach as for $\|D\|$, but the expression in (B3) would be multiplied by

$$[1 + L|\lambda|\Lambda + (L|\lambda|\Lambda)^2/2 + \ldots], \tag{B8}$$

for the exact exponential. That is equivalent to replacing the power with $2L5^{k-1} + L$, so one can give the upper bound on the order-s term as

$$\frac{(2\times 5^{k-1}+1)^s(L|\lambda|\Lambda)^s}{s!}. \tag{B9}$$

Therefore, replacing λ with $\lambda/2$, we can upper bound the size of the terms in $V^\dagger D + DV^\dagger$ by summing twice Eq. (B9) to give

$$A \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!}\exp[(5^{k-1}+1/2)|\lambda|L\Lambda]. \tag{B10}$$

Note that it is trivially true that $\|D\| \leqslant A/2$ because the sum of the magnitudes of the terms in $V^\dagger D + DV^\dagger$ upper bounds $\|V^\dagger D + DV^\dagger\| \geqslant 2\|D\|$. ■

APPENDIX C: ERROR BOUNDS BETWEEN THE MODIFIED RANDOMIZED FORMULA AND IDEAL UNITARY

When we obtain the explicit form of the formula in Sec. III A, we use Lemma 1 to bound the accuracy of the modified randomized product formula. Next, the proof is split into two parts. First, we prove the distance between each sampled unitary and the target unitary in Lemma 4. Then the bound of the distance between the average evolution and the target unitary is proved in Lemma 5. Combining Lemmas 4 and 5, we prove Theorem 1.

Lemma 4. (*Find the value of a for Theorem 1*). For any sampled unitary in $\{\widetilde{U}_{h,l}\}$, we have the bound

$$\left\| \exp\left(\lambda \sum_{j=1}^{L} H_j\right) - \widetilde{U}_{h,l} \right\| \leqslant 4\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda]. \tag{C1}$$

Lemma 5. (*Find the value of b for Theorem 1*). The distance between S^{avg}_{4k+1} and V is bounded as

$$\left\|S^{\text{avg}}_{4k+1}(\lambda) - V(\lambda)\right\| \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{4k+2}}{(4k+2)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda] + \frac{A^2}{2}\exp(A) + 3\|D\|^2 + 2\|D\|^3, \tag{C2}$$

where

$$\|D\| \leqslant \frac{(5^{k-1}|\lambda|L\Lambda)^{2k+1}}{(2k+1)!} \exp\left(5^{k-1}|\lambda|L\Lambda\right) + \frac{(|\lambda|L\Lambda/2)^{2k+1}}{(2k+1)!} \exp\left(|\lambda|L\Lambda/2\right) \tag{C3}$$

and

$$A \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda]. \tag{C4}$$

Given these lemmas, we can prove Theorem 1 as follows.

1. Proof of Theorem 1

Proof. Using the result in Lemma 4, and the upper bound on A, the equation $\|V - \widetilde{U}_{h,l}\| \leqslant a$ in Lemma 1 can be satisfied with a as in (14). Then, using Lemma 5, the condition $\|V - \sum_{h,l} p_{h,l}\widetilde{U}_{h,l}\| \leqslant b$ in Lemma 1 can be satisfied with b as in (15). There we have replaced $\|D\|$ with $A/2$ for simplicity because $\|D\| \leqslant A/2$. Therefore, we can use Lemma 1 to provide the bound $\|\mathcal{V}(\lambda) - \mathcal{E}(\lambda)\|_\diamond \leqslant a^2 + 2b$ required for Theorem 1. ■

2. Proof of Lemma 4

There are two major steps in this proof. We first explicitly express $V(\lambda) - \widetilde{U}_{h,l}(\lambda)$ as the summation of three parts, where $\widetilde{U}_{h,l}$ is the sampled unitary in $\{\widetilde{U}_{h,l}\}$. Then we individually calculate the norm of these three parts with the aid of Lemma 3. When we have their norms, we complete the proof by using triangle inequality.

Proof. The distance between the target unitary V and $\widetilde{U}_{h,l} = S_{2k}U_h^{(l)}S_{2k}$ can be upper bounded as

$$\begin{aligned}
&\left\| \exp\left(\lambda \sum_{j=1}^{L} H_j\right) - S_{2k}U_h^{(l)}S_{2k} \right\| \\
&= \left\| \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) - S_{2k}U_h^{(l)}S_{2k} \right\| \\
&\leqslant \left\| \left[\exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) - S_{2k} \right] \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) \right\| \\
&\quad + \left\| S_{2k}\left[\mathbb{1} - U_h^{(l)}\right] \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) \right\| \\
&\quad + \left\| S_{2k}U_h^{(l)} \left[\exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) - S_{2k} \right] \right\| \\
&\leqslant 2\left\| \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) - S_{2k} \right\| + \left\| \mathbb{1} - U_h^{(l)} \right\|.
\end{aligned} \tag{C5}$$

Using the expression for $U_h^{(l)}$ above, we have

$$\begin{aligned}
\left\| \mathbb{1} - U_h^{(l)} \right\| &= \left\| \mathbb{1} - \exp\left(\alpha_{h,l}H_h^{(l)}\right) \right\| \\
&\leqslant \left\| \alpha_{h,l}H_h^{(l)} \right\| = A,
\end{aligned} \tag{C6}$$

using the expressions for $\alpha_{h,l}$ and A in (38) and (41). We are considering the case where λ is imaginary so $\alpha_{h,l}$ is as well, which gives the second line above. Thus this error is equal to double the error of S_{2k} on $\lambda/2$ plus A,

$$\left\| \exp\left(\lambda \sum_{j=1}^{L} H_j\right) - S_{2k}U_h^{(l)}S_{2k} \right\| \leqslant 2\|D\| + A. \tag{C7}$$

From the results in Lemma 3 in Appendix B, we can bound the quantities $\|D\|$ and A as

$$\begin{aligned}
\|D\| &= \left\| \exp\left(\frac{\lambda}{2} \sum_{j=1}^{L} H_j\right) - S_{2k} \right\| \\
&\leqslant \frac{(5^{k-1}|\lambda|L\Lambda)^{2k+1}}{(2k+1)!} \exp\left(5^{k-1}|\lambda|L\Lambda\right) \\
&\quad + \frac{(|\lambda|L\Lambda/2)^{2k+1}}{(2k+1)!} \exp\left(|\lambda|L\Lambda/2\right)
\end{aligned} \tag{C8}$$

and

$$A \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda]. \tag{C9}$$

This gives the bound

$$\begin{aligned}
&\left\| \exp\left(\lambda \sum_{i=1}^{L} H_i\right) - S_{2k} U_h^{(l)} S_{2k} \right\| \\
&\leqslant 2\frac{(5^{k-1}|\lambda|L\Lambda)^{2k+1}}{(2k+1)!} \exp(5^{k-1}|\lambda|L\Lambda) \\
&\quad + 2\frac{(|\lambda|L\Lambda/2)^{2k+1}}{(2k+1)!} \exp\left(|\lambda|L\Lambda/2\right) \\
&\quad + 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda] \\
&\leqslant 4\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{2k+1}}{(2k+1)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda].
\end{aligned} \tag{C10}$$

■

3. Proof of Lemma 5

There are two steps in the proof of Lemma 5. First of all, we expand $S_{4k+1}^{\text{avg}}(\lambda)$, and this gives us the difference between $S_{4k+1}^{\text{avg}}(\lambda)$ and $V(\lambda)$. Next, we can bound the distance between $S_{4k+1}^{\text{avg}}(\lambda)$ and $V(\lambda)$ by using the triangle inequality. After we have the bound of these individual terms, we prove Lemma 5.

Proof. We explicitly expand S_{4k+1}^{avg} as

$$\begin{aligned}
&\sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} S_{2k} U_h^{(l)} S_{2k} \\
&= \sum_{l\in\gamma}\sum_{h=1}^{L_l} \frac{|\epsilon_{h,l}|}{A} S_{2k}\left[\mathbb{1} + \alpha_{h,l} H_h^{(l)} + \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j\right] S_{2k} \\
&= S_{2k}\left[\mathbb{1} - \sum_{l\in\gamma}\sum_{h=1}^{L_l}\left(\frac{\lambda}{2}\right)^l \beta_h^{(l)} H_h^{(l)}\right] S_{2k} \\
&\quad + S_{2k}\left[\sum_{l\in\gamma}\sum_{h=1}^{L_l} \frac{|\epsilon_{h,l}|}{A} \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j\right] S_{2k} \\
&= S_{2k}(\mathbb{1} - V^\dagger D - DV^\dagger) S_{2k} \\
&\quad + S_{2k}\left[\sum_{l\in\gamma}\sum_{h=1}^{L_l} \frac{|\epsilon_{h,l}|}{A} \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j\right] S_{2k} \\
&\quad + S_{2k}[R_{4k+1}(V^\dagger D + DV^\dagger)] S_{2k},
\end{aligned} \tag{C11}$$

where we define $R_{4k+1}(V^\dagger D + DV^\dagger)$ as the remainder of $V^\dagger D + DV^\dagger$ up to order $4k+1$. Next, note that the error in $S_{2k}(I - V^\dagger D - DV^\dagger)S_{2k}$ can be bounded as

$$\begin{aligned}
&\|(\mathbb{1} - V^\dagger D - DV^\dagger) - (\mathbb{1} + V^\dagger D)^{-1}(\mathbb{1} + DV^\dagger)^{-1}\| \\
&\quad = \|(\mathbb{1} + V^\dagger D)(\mathbb{1} - V^\dagger D - DV^\dagger)(\mathbb{1} + DV^\dagger) - \mathbb{1}\| \\
&\quad = \|V^\dagger DV^\dagger D + V^\dagger DDV^\dagger + DV^\dagger DV^\dagger \\
&\qquad + V^\dagger DV^\dagger DDV^\dagger - V^\dagger DDV^\dagger DV^\dagger\| \qquad \text{(C12)} \\
&\quad \leqslant 3\|D\|^2 + 2\|D\|^3. \qquad \text{(C13)}
\end{aligned}$$

Now we use the triangle bound to have

$$\begin{aligned}
&\left\| \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} S_{2k} U_h^{(l)} S_{2k} - V^2(\lambda/2) \right\| \\
&\quad \leqslant \left\| S_{2k}\left[\sum_{l\in\gamma}\sum_{h=1}^{L_l} \frac{|\epsilon_{h,l}|}{A} \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j\right] S_{2k} \right\| \qquad \text{(C14)} \\
&\qquad + \|S_{2k}[R_{4k+1}(V^\dagger D + DV^\dagger)] S_{2k}\| + 3\|D\|^2 + 2\|D\|^3. \qquad \text{(C15)}
\end{aligned}$$

Next, we bound each norm individually. Among Eq. (C14), we use some standard properties of norms, the definitions in Eqs. (38), (40), and (41), to have

$$\begin{aligned}
&\left\| S_{2k}\left[\sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j\right] S_{2k} \right\| \\
&\quad \leqslant \|S_{2k}\| \left\| \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} \sum_{j=2}^{\infty} \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j \right\| \|S_{2k}\| \\
&\quad \leqslant \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} \sum_{j=2}^{\infty} \left\| \frac{1}{j!}\left(\alpha_{h,l} H_h^{(l)}\right)^j \right\| \\
&\quad = \sum_{j=2}^{\infty} \frac{A^j}{j!} \leqslant \frac{A^2}{2}\exp(A).
\end{aligned} \tag{C16}$$

In the second-to-last line, we have used the fact that the sum over probabilities is equal to 1.

For the norm in Eq. (C15), using some basic properties of norms, we have

$$\begin{aligned}
&\|S_{2k}[R_{4k+1}(V^\dagger D + DV^\dagger)] S_{2k}\| \\
&\quad \leqslant \|S_{2k}\| \|R_{4k+1}(V^\dagger D + DV^\dagger)\| \|S_{2k}\| \\
&\quad \leqslant \|R_{4k+1}(V^\dagger D + DV^\dagger)\|.
\end{aligned} \tag{C17}$$

This can be bounded using Eq. (B9), and summing from $s = 4k+2$ to infinity with λ replaced with $\lambda/2$ for the half interval to give

$$\begin{aligned}
&2\sum_{s=4k+2}^{\infty} \frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^s}{s!} \\
&\quad \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{4k+2}}{(4k+2)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda].
\end{aligned} \tag{C18}$$

As a result, we have

$$\begin{aligned}
&\left\| \sum_{l\in\gamma}\sum_{h=1}^{L_l} p_{h,l} S_{2k} U_h^{(l)} S_{2k} - V^2(\lambda/2) \right\| \\
&\quad \leqslant 2\frac{[(5^{k-1}+1/2)|\lambda|L\Lambda]^{4k+2}}{(4k+2)!} \exp[(5^{k-1}+1/2)|\lambda|L\Lambda] \\
&\qquad + \frac{A^2}{2}\exp(A) + 3\|D\|^2 + 2\|D\|^3,
\end{aligned} \tag{C19}$$

where we bound $\|D\|$ and A in Lemma 3. ■

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