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On the Efficiency of Quantum Algorithms for Hamiltonian Simulation

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Abstract We study algorithms simulating a system evolving with Hamiltonian $H = \sum_{j=1}^{m} H_j$, where each of the H_j, $j = 1, \ldots, m$, can be simulated efficiently. We are interested in the cost for approximating e^{-iHt}, $t \in \mathbb{R}$, with error ε. We consider algorithms based on high order splitting formulas that play an important role in quantum Hamiltonian simulation. These formulas approximate e^{-iHt} by a product of exponentials involving the H_j, $j = 1, \ldots, m$. We obtain an upper bound for the number of required exponentials. Moreover, we derive the order of the *optimal* splitting method that minimizes our upper bound. We show significant speedups relative to previously known results.

Keywords Quantum simulation, complexity, Hamiltonian evolution, splitting methods, order of convergence

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1 Introduction

Simulating quantum systems using classical computers appears to be a very difficult problem. The number of parameters describing the quantum states grows exponentially with the system size and so does the computational cost of the best classical deterministic algorithms known. In some cases classical randomized algorithms have been used to overcome these difficulties, however, randomized algorithms also have limitations. As an alternative to simulation with a classical computer Feynman proposed simulation with a quantum computer. He conjectured that quantum computers might be able to carry the simulation more efficiently than classical computers. For an overview of quantum simulation see, e.g., [1–4].

In the Hamiltonian simulation problem one is given a Hamiltonian H, $t \in \mathbb{R}$ and an accuracy demand ε and the goal is to derive an algorithm approximating the unitary operator e^{-iHt} with error at most ε. The size of the quantum circuit

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realizing the algorithm is its cost. Assuming that H is a matrix of size $2^q \times 2^q$ the algorithm is efficient if its cost is a polynomial in q, t and ε^{-1}.

Lloyd [2] showed that local Hamiltonians can be simulated efficiently on a quantum computer. About the same time, Zalka [18,19] showed that many-particle systems can be simulated efficiently on a quantum computer. Later, Aharonov and Ta-Shma [6] generalized Lloyd's results to sparse Hamiltonians. We note that Hamiltonian simulations is also related to adiabatic evolution and quantum walks [7–11].

Berry et al. [5] extended the complexity results of [6] for sparse Hamiltonians. They assume that the Hamiltonian H is given by an "oracle"(a "black-box") and that H can be decomposed efficiently by a quantum algorithm using oracle calls into a sum of Hamiltonians H_j, $j = 1, \dots, m$, that individually can be simulated efficiently. They approximate e^{-Ht} with error ε by a sequence of N unitary operators of the form $e^{-iH_{j_\ell} t_{j_\ell}}$, $\ell = 1, \dots, N$. The cost of the simulation is the total number of oracle calls. All the unitary operators in the sequence have to be considered in the simulation, the one after the other. The algorithm has to make oracle calls to each Hamiltonian appearing in the sequence and to simulate it. Each oracle call to any H_j is simulated by making oracle calls to H; see [5, Sec. 5] for details. Thus the total number of oracle calls is proportional to N, although it is not equivalent since there can be overhead in implementing each $e^{-iH_{j_\ell} t_{j_\ell}}$, $\ell = 1, \dots, N$.

In particular, let $H = \sum_{j=1}^m H_j$, where $e^{-iH_j t}$, $t \in \mathbb{R}$, can be implemented efficiently, and the H_j do not commute, $j = 1, \dots, m$. Consider algorithms approximating e^{-iHt}, $t \in \mathbb{R}$, that are obtained from products of exponentials having the form

$$\prod_{l=1}^{N} e^{-iH_{j_l} t_{j_l}}, \tag{1}$$

for suitable $t_{j_l} \in \mathbb{R}$, where $j_l \in \{1, \dots, m\}$. The cost of the simulation of H is proportional to number of exponentials, N, so that

$$\left\| e^{-iHt} - \prod_{l=1}^{N} e^{-iH_{j_l} t_{j_l}} \right\| \le \varepsilon.$$

Berry et al. [5] use Suzuki's [13,14] *high order splitting formulas* to derive (1). They obtain an upper bound for N, which among other factors depends on ε and the order of the splitting formula. They obtain the order of the splitting method minimizing their upper bound.

Recall that splitting formulas such as the Lie-Trotter formula

$$\lim_{n \to \infty} \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \right)^n = e^{-i(H_1 + H_2)t},$$

have been extensively used in quantum simulation. From this we have a second order approximation

$$e^{-i(H_1+H_2)\Delta t} = e^{-iH_1 \Delta t} e^{-iH_2 \Delta t} + O(|\Delta t|^2).$$

A third order approximation is given by the Strang splitting formula

$$e^{-i(H_1+H_2)\Delta t} = e^{-iH_1 \Delta t/2} e^{-iH_2 \Delta t} e^{-iH_1 \Delta t/2} + O(|\Delta t|^3).$$

Suzuki [13,14] uses recursive modifications of this approximation to derive formulas of order $2k+1$, for $k = 1, 2, \dots$.

We also use Suzuki's formulas, improve the upper bound of N shown in [5] and obtain the order of the splitting method that minimizes our upper bound.

2 Overview of the results

In approximating e^{-iHt} by a product of the form (1), where $H = \sum_{j=1}^{m} H_j$, the relative magnitudes of the norms of the H_j are important. The approximation error depends on them and since we want accuracy ε this affects the number $N = N(\varepsilon)$ of required exponentials in the product. (Note that we have assumed the H_j do not commute.)

The estimates of N that we will be presenting hold for Hermitian matrices or bounded Hermitian operators so that $\|H_j\| < \infty$, $j = 1, \dots, m$. (The norm $\|\cdot\|$ is a matrix or operator norm induced by the norm of the underlying Hilbert space.)

Consider the Hamiltonians indexed with respect to the magnitude of their norms $\|H_1\| \geq \|H_2\| \geq \cdots \geq \|H_m\|$. Then the number of necessary exponentials N generally depends on H_1, but it must also depend explicitly on H_2 since only one exponential should suffice for the simulation if $\|H_2\| \to 0$. This observation is particularly important for the simulation of systems in physics and chemistry. To see this, suppose $m = 2$ and that H_1 is a discretization of the negative Laplacian $-\Delta$, while H_2 is a discretization of a uniformly bounded potential. Then $e^{-iH_1 t_1}$ and $e^{-iH_2 t_2}$ can be implemented efficiently for any t_1, t_2, and $\|H_2\| \ll \|H_1\|$. We will see that, not only in this case but in general, the number of exponentials is proportional to both $\|H_1\|$ and $\|H_2\|$, i.e., the Hamiltonian of the second largest norm plays an important role.

Let ε be sufficiently small. The previously known bound for the number of exponentials, according to [5] (see Lemma 1 and Theorem 1 in that paper), is

$$N \leq N_{\text{prev}} := m 5^{2k} (m\|H_1\|t)^{1+\frac{1}{2k}} \varepsilon^{-1/(2k)}, \tag{2}$$

where the splitting formula is of order $2k+1$. This bound does not properly reflect the dependence on H_2. A similar estimate follows from [15] that deals with a more general Hamiltonian simulation problem. Modulo constants, it improves the dependence on k of the number of exponentials by replacing 5^{2k} with $(25/3)^k$ in the bound above. However, the important role of H_2 is not reflected by the approach of [15] either.

Performing a more detailed analysis of the approximation error by high order splitting formulas, it is possible to improve the bounds for N. The new estimates lead to splitting methods of significantly lower order which greatly reduces the cost of the algorithms. Our estimates improve those of [5, 15]. We compare our results to those of [5] which also deals with the determination of the optimal k that minimizes the bound for N.

We now summarize our results. Recall that the H_j can be implemented efficiently but do not commute and $\|H_1\| \geq \|H_2\| \geq \cdots \|H_m\|$. We show the following:

1. A new bound for the number of exponentials N, given by
$$N \leq N_{\text{new}} := 2(2m-1)\; 5^{k-1} \|H_1\| t \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{4me}{3} \left(\frac{5}{3}\right)^{k-1}.$$
2. A speedup factor of
$$\frac{N_{\text{new}}}{N_{\text{prev}}} \leq \frac{2}{3^k} \left(\frac{4e\|H_2\|}{\|H_1\|}\right)^{1/2k}.$$
3. We show that the *optimal* k^*_{new} that minimizes N_{new} is
$$k^*_{\text{new}} := \text{round}\left(\sqrt{\frac{1}{2}\log_{25/3} \frac{4emt\|H_2\|}{\varepsilon}}\right).$$

On the other hand, from [5] the bound for $N_{\rm prev}$ is minimized for

$$k^*_{\rm prev} = \text{round}\left(\frac{1}{2}\sqrt{\log_5 \frac{m\|H_1\|t}{\varepsilon} + 1}\right).$$

4. For $k^*_{\rm new}$ the value of $N_{\rm new}$ satisfies

$$N^*_{\rm new} \le \frac{8}{3}\,(2m-1)\,emt\,\|H_1\|\; e^{2\sqrt{\frac{1}{2}\ln\frac{25}{3}\ln\frac{4emt\|H_2\|}{\varepsilon}}}.$$

For $k^*_{\rm prev}$ the value of $N_{\rm prev}$ is

$$N^*_{\rm prev} = 2m^2\|H_1\|t\cdot e^{2\sqrt{\ln 5\ln(m\|H_1\|t/\epsilon)}}.$$

Hence

$$\frac{N^*_{\rm new}}{N^*_{\rm prev}} \le \frac{8\,e}{3}\,e^{2\left(\sqrt{\frac{1}{2}\ln\frac{25}{3}\ln\frac{4emt\|H_2\|}{\varepsilon}} - \sqrt{\ln 5\ln\frac{m\|H_1\|t}{\varepsilon}}\right)}.$$

Finally, we illustrate our results using the example we mentioned earlier involving the simulation of $H = -\Delta + V$, where Δ is the Laplacian and V is a bounded potential. Suppose this problem is discretized on a grid with mesh size h. The resulting matrix is $H_h = -\Delta_h + V_h$, where Δ_h and V_h denote the discretizations of the Laplacian and the potential, respectively. Then $\|\Delta_h\|$ is proportional to h^{-2} while $\|V_h\|$ is uniformly bounded. For a fine discretization $\|V_h\| \ll \|\Delta_h\|$.

Observe that $k^*_{\rm new}$ depends on $\|V_h\|$, which is uniformly bounded, and not on $\|\Delta_h\|$. The value of $k^*_{\rm new}$ is independent of h. Hence, the splitting formula does not change with h.

On the other hand, $k^*_{\rm prev}$ depends on $\|\Delta_h\|$ and therefore on h^{-2}. It will increase if h is to become smaller. Thus, the corresponding splitting formula changes with h, a costly and unnecessary consequence.

If k is to be kept fixed, then the ratio $N_{\rm new}/N_{\rm prev}$ is proportional to $h^{-1/k}$. (The same is true for our estimate relative to the one that follows from [15].) This speedup can be significant in practice. Consider, for instance, $h = 10^{-8}$ and a small value of k. For the simulation of $e^{-iH_h t}$ using a product of exponentials obtained by multiple applications of the Strang splitting formula, where $k = 1$ and it has order 3, our results lead to a speedup proportional to 10^8. Similarly, for a method of order 5, i.e., $k = 2$, the speedup is proportional to 10^4.

3 Splitting methods for simulating the sum of two Hamiltonians

We begin this section by discussing the simulation of

$$e^{-i(H_1+H_2)t},$$

where H_1, H_2 are given Hamiltonians. Restricting the analysis to $m = 2$ will allow us to illustrate the main idea in our approach while avoiding the rather complicated notation needed in the general case, for $m \ge 2$. The simulation of the Schrödinger equation of a p-particle system, where H_1 is obtained from the Laplacian operator and H_2 is the potential, requires one to consider an evolution operator that has the form above; see [3].

In the next section we deal with the more general simulation problem involving a sum of m Hamiltonians, $H_1, \ldots, H_m$, as Berry et al. [5] did, and we will show how to improve their complexity results.

Suzuki proposed methods for decomposing exponential operators in a number of papers [13,14]. For sufficiently small Δt, starting from the formula

$$S_2(H_1, H_2, \Delta t) = e^{-iH_1\Delta t/2} e^{-iH_2\Delta t} e^{-iH_1\Delta t/2},$$

and proceeding recursively, Suzuki defines

$$\begin{aligned} &S_{2k}(H_1, H_2, \Delta t) \\ =&[S_{2k-2}(H_1, H_2, p_k\Delta t)]^2 S_{2k-2}(H_1, H_2, (1-4p_k)\Delta t)[S_{2k-2}(H_1, H_2, p_k\Delta t)]^2, \end{aligned}$$

for $k = 2, 3, \cdots$, where $p_k = (4 - 4^{1/(2k-1)})^{-1}$, and then proves that

$$\left\| e^{-i(H_1+H_2)\Delta t} - S_{2k}(H_1, H_2, \Delta t) \right\| = O(|\Delta t|^{2k+1}). \tag{3}$$

Suzuki was particularly interested in the order of his method, which is $2k+1$, and did not address the size of the implied asymptotic factors in the big-O notation. However, these factors depend on the norms of H_1 and H_2 and can be very large, when H_1 and H_2 do not commute. For example, recall that when H_1 is obtained from the discretization of the Laplacian operator with mesh size h, $\|H_1\|$ grows as h^{-2}. For $h = \varepsilon$, we get $\|H_1\| = O(\frac{1}{\varepsilon^2})$. Hence, for fine discretizations $\|H_1\|$ is huge, and severely affects the error bound above.

Suppose $\|H_1\| \geq \|H_2\|$. Since

$$e^{-i(H_1+H_2)t} = e^{-i(\mathcal{H}_1+\mathcal{H}_2)\|H_1\|t},$$

where $\mathcal{H}_j = H_j/\|H_1\|$, for $j = 1, 2$, we can consider the simulation problem for $\mathcal{H}_1 + \mathcal{H}_2$ with an evolution time $\tau = \|H_1\|t$.

Unwinding the recurrence in Suzuki's construction yields

$$S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t) = \prod_{\ell=1}^{K} S_2(\mathcal{H}_1, \mathcal{H}_2, z_\ell \Delta t) = \prod_{\ell=1}^{K} \left[e^{-i\mathcal{H}_1 z_\ell \Delta t/2} e^{-i\mathcal{H}_2 z_\ell \Delta t} e^{-i\mathcal{H}_1 z_\ell \Delta t/2} \right], \tag{4}$$

where $K = 5^{k-1}$ and each z_ℓ is defined according to the recursive scheme, $\ell = 1, \ldots, K$. In particular, $z_1 = z_K = \prod_{r=2}^{k} p_r$, and for the intermediate values of ℓ the z_ℓ is a product of $k-1$ factors and has the form $z_\ell = \prod_{r\in I_0} p_r \prod_{r\in I_1}(1-4p_r)$, where the products are over the index sets I_0, I_1 defined by traversing the corresponding to ℓ path of the recursion tree.

Let $q_r = \max\{p_r, 4p_r - 1\}$, $r \geq 2$. Then $\{q_r\}$ is a decreasing sequence of positive numbers and from [15, p. 18] we have that

$$\frac{3}{3^k} \leq \prod_{r=2}^{k} q_r \leq \frac{4k}{3^k}.$$

Thus

$$|z_\ell| \leq \frac{4k}{3^k} \quad \text{for all } \ell = 1, \ldots, K. \tag{5}$$

Equation (4) can be expressed in the more compact form which we use to simplify the notation. Namely,

$$S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t) = e^{-i\mathcal{H}_1 s_0 \Delta t} e^{-i\mathcal{H}_2 z_1 \Delta t} e^{-i\mathcal{H}_1 s_1 \Delta t} \cdots e^{-i\mathcal{H}_2 z_K \Delta t} e^{-i\mathcal{H}_1 s_K \Delta t}, \tag{6}$$

where $s_0 = z_1/2$, $s_j = (z_j + z_{j+1})/2$, $j = 1, \ldots, K-1$, and $s_K = z_K/2$. Observe that $\sum_{j=0}^{K} s_j = 1$, $\sum_{j=1}^{K} z_j = 1$.

We need to bound $\sigma_k = \sum_{j=0}^K |s_j| + \sum_{j=1}^K |z_j|$ from above. From (5) we have

$$\sum_{j=1}^{K} |z_j| \le \frac{4k5^{k-1}}{3^k},$$

and also

$$\sum_{j=0}^{K} |s_j| \le \frac{4k5^{k-1}}{3^k}.$$

Thus

$$\sigma_k \le \frac{8}{3}k\left(\frac{5}{3}\right)^{k-1} =: c_k \quad \text{for } k \ge 1. \tag{7}$$

(The above trivially holds for $k = 1$.)

Expanding each exponential in (6) we obtain

$$\begin{aligned}
&S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t)\\
=&(I + \mathcal{H}_1 s_0(-i\Delta t) + \frac{1}{2}\mathcal{H}_1^2 s_0^2(-i\Delta t)^2 + \cdots + \frac{1}{k!}\mathcal{H}_1^k s_0^k(-i\Delta t)^k + \cdots)\\
&\cdot (I + \mathcal{H}_2 z_1(-i\Delta t) + \frac{1}{2}\mathcal{H}_2^2 z_1^2(-i\Delta t)^2 + \cdots + \frac{1}{k!}\mathcal{H}_2^k z_1^k(-i\Delta t)^k + \cdots)\\
&\cdot (I + \mathcal{H}_1 s_1(-i\Delta t) + \frac{1}{2}\mathcal{H}_1^2 s_1^2(-i\Delta t)^2 + \cdots + \frac{1}{k!}\mathcal{H}_1^k s_1^k(-i\Delta t)^k + \cdots)\\
&\cdots\\
&\cdot (I + \mathcal{H}_2 z_K(-i\Delta t) + \frac{1}{2}\mathcal{H}_2^2 z_K^2(-i\Delta t)^2 + \cdots + \frac{1}{k!}\mathcal{H}_2^k z_K^k(-i\Delta t)^k + \cdots)\\
&\cdot (I + \mathcal{H}_1 s_K(-i\Delta t) + \frac{1}{2}\mathcal{H}_1^2 s_K^2(-i\Delta t)^2 + \cdots + \frac{1}{k!}\mathcal{H}_1^k s_K^k(-i\Delta t)^k + \cdots).
\end{aligned} \tag{8}$$

After carrying out the multiplications we see that S_{2k} is a sum of terms that has the form

$$\frac{s_0^{\alpha_0}s_1^{\alpha_1}\cdots s_K^{\alpha_K} z_1^{\beta_1}\cdots z_K^{\beta_K}}{\alpha_0!\alpha_1!\cdots\alpha_K!\beta_1!\cdots\beta_K!}\mathcal{H}_1^{\alpha_0}\mathcal{H}_2^{\beta_1}\mathcal{H}_1^{\alpha_1}\cdots\mathcal{H}_2^{\beta_K}\mathcal{H}_1^{\alpha_K}(-i\Delta t)^{\sum_{i=0}^K \alpha_i + \sum_{j=1}^K \beta_j}, \tag{9}$$

where the $\alpha_0, \alpha_1, \cdots, \alpha_K$ and the $\beta_1, \cdots, \beta_K$ are obtained by multiplying the denominators in the expansion of the exponentials.

The terms that do not contain $\mathcal{H}_2$ are those for which $\beta_1 = \beta_2 = \cdots = \beta_K = 0$, and their sum is

$$\begin{aligned}
&\sum_{\alpha_0,\alpha_1,\cdots,\alpha_K} \frac{s_0^{\alpha_0}s_1^{\alpha_1}\cdots s_K^{\alpha_K}}{\alpha_0!\alpha_1!\cdots\alpha_K!}\mathcal{H}_1^{\sum_{j=0}^K \alpha_j}(-i\Delta t)^{\sum_{j=0}^K \alpha_j}\\
&= \sum_{\alpha_0} \frac{1}{\alpha_0!}\mathcal{H}_1^{\alpha_0}(-is_0\Delta t)^{\alpha_0} \cdot \sum_{\alpha_1} \frac{1}{\alpha_1!}\mathcal{H}_1^{\alpha_1}(-is_1\Delta t)^{\alpha_1} \cdot \cdots \cdot \sum_{\alpha_K} \frac{1}{\alpha_K!}\mathcal{H}_1^{\alpha_K}(-is_K\Delta t)^{\alpha_K}\\
&= \prod_{j=0}^{K} e^{-i\mathcal{H}_1 s_j \Delta t} = \exp(-i\sum_{j=0}^{K}\mathcal{H}_1 s_j \Delta t) = \exp(-i\mathcal{H}_1\Delta t).
\end{aligned} \tag{10}$$

On the other hand, consider

$$e^{-i(\mathcal{H}_1+\mathcal{H}_2)\Delta t} = I + (-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) + \cdots + \frac{1}{k!}(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t)^k + \cdots. \tag{11}$$

The terms that do not contain $\mathcal{H}_2$ sum to

$$\sum_{k=0}^{\infty} \frac{1}{k!} \mathcal{H}_1^k (-i\Delta t)^k = e^{-i\mathcal{H}_1 \Delta t}. \tag{12}$$

Let us now consider the bound in (3). Subtracting (8) from (11) the terms that do not contain $\mathcal{H}_2$ cancel out. Therefore, the error is proportional to $\|\mathcal{H}_2\||\Delta t|^{2k+1}$, i.e. it depends on the ratio $\|H_2\|/\|H_1\|$ of the norms of the original Hamiltonians. This fact will be used to improve the error and complexity results of Berry et al. [5]

Lemma 1 *For $k \in \mathbb{N}$, $c_k|\Delta t| \le k+1$ (see, Eq. 7) and $\|\mathcal{H}_2\| \le \|\mathcal{H}_1\| = 1$ we have*

$$\| \exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) - S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t)\| \le \frac{4\|\mathcal{H}_2\|}{(2k+1)!} (c_k|\Delta t|)^{2k+1}. \tag{13}$$

Proof For notational convenience we use $S_{2k}(\Delta t)$ to denote $S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \Delta t)$. Consider

$$\exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t) - S_{2k}(\Delta t) = \sum_{l=2k+1}^{\infty} \big[R_l(\Delta t) - T_l(\Delta t)\big], \tag{14}$$

where $R_l(\Delta t)$ is the sum of all terms in $\exp(-i(\mathcal{H}_1 + \mathcal{H}_2)\Delta t)$ corresponding to Δt^l and $T_l(\Delta t)$ is the sum of all terms in $S_{2k}(\Delta t)$ corresponding to Δt^l. Moreover, we know that the terms with only $\mathcal{H}_1$ cancel out. Hence, we can ignore the terms in $T_l(\Delta t)$ and $R_l(\Delta t)$ that contain only $\mathcal{H}_1$ (and not $\mathcal{H}_2$) as a factor. It follows that

$$R_l(\Delta t) = \frac{1}{l!}(\mathcal{H}_1 + \mathcal{H}_2)^l (-i\Delta t)^l - \frac{1}{l!}\mathcal{H}_1^l (-i\Delta t)^l. \tag{15}$$

Then

$$\|R_l(\Delta t)\| \le \frac{1}{l!} 2^l \|\mathcal{H}_2\||\Delta t|^l, \tag{16}$$

since there are $2^l - 1$ terms, and they are bounded by $\frac{1}{l!}\|\mathcal{H}_2\||\Delta t|^l$.

Now consider the terms in $T_l(\Delta t)$. From (8,9)

$$T_l(\Delta t) = \sum \frac{s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}}{\alpha_0!\alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} \mathcal{H}_1^{\alpha_0} \mathcal{H}_2^{\beta_1} \mathcal{H}_1^{\alpha_1} \cdots \mathcal{H}_2^{\beta_K} \mathcal{H}_1^{\alpha_K} (-i\Delta t)^l, \tag{17}$$

where the summation is over the set of tuples $(\alpha_0, \alpha_1, \cdots, \alpha_K)$ and $(\beta_1, \cdots, \beta_K)$ that satisfy $\sum_{i=0}^K \alpha_i + \sum_{i=1}^K \beta_i = l$ and $\sum_{i=1}^K \beta_i \ne 0$; the latter condition excludes terms containing $\mathcal{H}_1$ alone. Since the norm of $\mathcal{H}_1^{\alpha_0} \mathcal{H}_2^{\beta_1} \mathcal{H}_1^{\alpha_1} \cdots \mathcal{H}_2^{\beta_K} \mathcal{H}_1^{\alpha_K}$ is at most $\|\mathcal{H}_2\|$, we have

$$\|T_l(\Delta t)\| \le \sum_{\sum_{i=0}^K \alpha_i + \sum_{i=1}^K \beta_i = l} \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0!\alpha_1! \cdots \alpha_K! \beta_1! \cdots \beta_K!} \|\mathcal{H}_2\||\Delta t|^l. \tag{18}$$

Note that we relaxed the condition $\sum_{i=1}^K \beta_i \ne 0$ since it does not affect the inequality.

To calculate the sum $\sum \frac{|s_0^{\alpha_0} s_1^{\alpha_1} \cdots s_K^{\alpha_K} z_1^{\beta_1} \cdots z_K^{\beta_K}|}{\alpha_0!\alpha_1!\cdots\alpha_K!\beta_1!\cdots\beta_K!}$, where $\sum_{i=0}^{K}\alpha_i + \sum_{i=1}^{K}\beta_i = l$, we first consider the following equation

$$\begin{aligned}
&\exp(|s_0\Delta t|)\exp(|z_1\Delta t|)\exp(|s_1\Delta t|)\cdots\exp(|z_K\Delta t|)\exp(|s_K\Delta t|)\\
&= \left(\sum_{\alpha_0=0}^{\infty}\frac{1}{\alpha_0!}|s_0\Delta t|^{\alpha_0}\right)\cdot\left(\sum_{\beta_1=0}^{\infty}\frac{1}{\beta_1!}|z_1\Delta t|^{\beta_0}\right)\cdot\left(\sum_{\alpha_1=0}^{\infty}\frac{1}{\alpha_1!}|s_1\Delta t|^{\alpha_0}\right)\cdots\\
&\qquad\cdots\cdot\left(\sum_{\beta_K=0}^{\infty}\frac{1}{\beta_K!}|z_K\Delta t|^{\beta_K}\right)\cdot\left(\sum_{\alpha_K=0}^{\infty}\frac{1}{\alpha_K!}|s_K\Delta t|^{\alpha_K}\right)\\
&= \sum_{p=0}^{\infty}\sum_{\sum\alpha_j+\sum\beta_j=p}\frac{|s_0^{\alpha_0}s_1^{\alpha_1}\cdots s_K^{\alpha_K}z_1^{\beta_1}\cdots z_K^{\beta_K}|}{\alpha_0!\alpha_1!\cdots\alpha_K!\beta_1!\cdots\beta_K!}|\Delta t|^p.
\end{aligned} \tag{19}$$

Hence $\sum_{\sum\alpha_j+\sum\beta_j=l}\frac{|s_0^{\alpha_0}s_1^{\alpha_1}\cdots s_K^{\alpha_K}z_1^{\beta_1}\cdots z_K^{\beta_K}|}{\alpha_0!\alpha_1!\cdots\alpha_K!\beta_1!\cdots\beta_K!}$ is the coefficient of $|\Delta t|^l$ in the equation above. Similarly,

$$\begin{aligned}
&\exp(|s_0\Delta t|)\exp(|z_1\Delta t|)\exp(|s_1\Delta t|)\cdots\exp(|z_K\Delta t|)\exp(|s_K\Delta t|)\\
&= \exp((\sum_{i=0}^{K}|s_i| + \sum_{i=1}^{K}|z_i|)|\Delta t|) = \exp(\sigma_k|\Delta t|)\\
&= \sum_{p=0}^{\infty}\frac{1}{p!}\sigma_k^p|\Delta t|^p,
\end{aligned} \tag{20}$$

Recall that the bound for σ_k given in Eq. (7). Thus the coefficient of $|\Delta t|^l$ is bounded from above by $\frac{1}{l!}c_k^l$. Therefore, we have

$$\|T_l(\Delta t)\| \le \frac{c_k^l}{l!}\|\mathcal{H}_2\||\Delta t|^l. \tag{21}$$

We combine Eq. (16), (21), to obtain

$$\begin{aligned}
&\|\exp((\mathcal{H}_1+\mathcal{H}_2)\Delta t) - S_{2k}(\Delta t)\|\\
\le&\sum_{l=2k+1}^{\infty}\|R_l(\Delta t) - T_l(\Delta t)\|\\
\le&\sum_{l=2k+1}^{\infty}\|R_l(\Delta t)\| + \|T_l(\Delta t)\|\\
\le&2\sum_{l=2k+1}^{\infty}\frac{c_k^l}{l!}\|\mathcal{H}_2\||\Delta t|^l\\
\le&\frac{2}{(2k+1)!}\|\mathcal{H}_2\||c_k\Delta t|^{2k+1}\left(1-\frac{c_k|\Delta t|}{2k+2}\right)^{-1}\\
\le&\frac{4}{(2k+1)!}\|\mathcal{H}_2\||c_k\Delta t|^{2k+1},
\end{aligned} \tag{22}$$

where the last two inequalities follow from the assumption $c_k|\Delta t| \le k+1$. and an estimate of the tail of the Poisson distribution; see, e.g., [16, Thm 1]. □

Theorem 1 *Let $1 \geq \varepsilon > 0$ be such that $8et\|H_2\| \geq \varepsilon$. The number N of exponentials for the simulation of $e^{-i(H_1+H_2)t}$ with accuracy ε is bounded as follows*

$$N \leq 3\, 5^{k-1} \left\lceil \|H_1\| t \left(\frac{8et\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{8e}{3} \left(\frac{5}{3}\right)^{k-1} \right\rceil ,$$

for any $k \in \mathbb{N}$, where $\|H_2\| \leq \|H_1\|$.

Proof Let $M = |\Delta t|^{-1}$. Then using Lemma 1 and $\mathcal{H}_j = H_j/\|H_1\|$, $j = 1, 2$, we obtain

$$\begin{aligned} \left\| e^{-i(H_1+H_2)t} - S_{2k}^{M\|H_1\|t}(\mathcal{H}_1, \mathcal{H}_2, 1/M) \right\| &\leq M\|H_1\|t \frac{4}{(2k+1)!} \|\mathcal{H}_2\| \left(\frac{c_k}{M}\right)^{2k+1} \\ &= 4t\|H_2\| \frac{c_k^{2k+1}}{(2k+1)!} \frac{1}{M^{2k}}. \end{aligned} \tag{23}$$

Recall that c_k is defined in (7) and is used in Lemma 1. For accuracy ε we obtain

$$M \geq \left(\frac{4t\|H_2\| c_k^{2k+1}}{\varepsilon (2k+1)!} \right)^{1/(2k)} .$$

We use Stirling's formula [17, p. 257] for the factorial function

$$(2k+1)! = \sqrt{2\pi}(2k+1)^{(2k+1)+1/2} e^{-(2k+1)+\theta/(12(2k+1))}, \quad 0 < \theta < 1,$$

which yields

$$[(2k+1)!]^{-1/(2k)} \leq e^{1+1/(2k)}/(2k+1). \tag{24}$$

It is easy to check that

$$c_k^{1/(2k)} \leq 2^{1+1/(2k)}.$$

Thus it suffices to take

$$M \geq \left(\frac{8et\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{2\, e\, c_k}{2k+1}.$$

So we define M to be lower bound of the expression above, i.e.,

$$M := \left(\frac{8et\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{2e\, c_k}{2k+1}.$$

It is easy to check that

$$\frac{2e}{2k+1}(k+1) \geq e,$$

which along with the condition $8et\|H_2\| \geq \varepsilon$ yields $M(k+1) \geq c_k$. This shows the assumptions of Lemma 1 are satisfied with this value of M.

From the recurrence relation the number of required exponentials to implement S_{2k} in one subinterval is no more than $3 \cdot 5^{k-1}$. We need to consider two cases concerning $M\|H_1\|t$. If $M\|H_1\|t \geq 1$, then the number of subintervals is $\lceil M\|H_1\|t \rceil$, i.e., we partition the entire time interval into an integer number of subintervals, each of length at most M^{-1}. The total number of required exponentials is bounded by $3 \cdot 5^{k-1} \lceil M\|H_1\|t \rceil$. Substituting the values of M and c_k we obtain the bound for N. In particular,

$$N \leq 3 \cdot 5^{k-1} \left\lceil \|H_1\| t \left(\frac{8et\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{8e}{3} \left(\frac{5}{3} \right)^{k-1} \right\rceil . \tag{25}$$

If $M\|H_1\|t < 1$, then Lemma 1 can be used with $\Delta t = \|H_1\|t$, since $\|H_1\|t \leq M^{-1}$ and we have already seen that M is such that the assumptions of Lemma 1 are satisfied. Thus

$$\begin{aligned} \left\| e^{-i(H_1+H_2)t} - S_{2k}(\mathcal{H}_1, \mathcal{H}_2, \|H_1\|t) \right\| &\leq \frac{4}{(2k+1)!} \|\mathcal{H}_2\| \left(c_k \|H_1\| t \right)^{2k+1} \\ &= 4t\|H_2\| \frac{c_k^{2k+1}}{(2k+1)!} (\|H_1\|t)^{2k} \leq 4t\|H_2\| \frac{c_k^{2k+1}}{(2k+1)!} (M)^{-2k} \leq \varepsilon, \end{aligned}$$

where the last inequality holds by definition of M. In this case the total number of exponentials is simply

$$N \leq 3 \cdot 5^{k-1}. \tag{26}$$

Combining (25) and (26) we obtain

$$N \leq 3 \cdot 5^{k-1} \left\lceil \|H_1\| t \left(\frac{8et\|H_2\|}{\varepsilon} \right)^{1/(2k)} \frac{8e}{3} \left(\frac{5}{3} \right)^{k-1} \right\rceil .$$

This completes the proof. $\square$

Remark 1 *Lemma 1 and Theorem 1 indicate that when $\|H_2\|t \ll \varepsilon$ then the number of exponentials N can be further improved. In this case it can be shown that high order splitting methods may lose their advantage. We do not pursue this direction in this paper since we assume that the H_j, $j = 1, \ldots, m$, are fixed and study N as $\varepsilon \to 0$.*

4 Splitting methods for simulating the sum of many Hamiltonians

In this section we deal with the simulation of

$$e^{-i \sum_{j=1}^m H_j t},$$

where H_j, $j = 1, \ldots, m$, $m \geq 2$, are given non-commuting Hamiltonians. The analysis and the conclusions are similar to those of the previous section where $m = 2$, but the proofs are much more complicated. This is the problem that Berry et al. [5] considered.

We use Suzuki's recursive construction once more [14]. In particular, for

$$S_2(H_1, \ldots, H_m, \Delta t) = \prod_{j=1}^{m} e^{-iH_j \Delta t/2} \prod_{j=m}^{1} e^{-iH_j \Delta t/2},$$

and

$$S_{2k}(H_1, \ldots, H_m, \Delta t) = [S_{2k-2}(p_k \Delta t)]^2 S_{2k-2}((1-4p_k)\Delta t)[S_{2k-2}(p_k \Delta t)]^2,$$

for $k = 2, 3, \ldots$, where for notational convenience we have used $S_{2k-2}(\Delta t)$ to denote $S_{2k-2}(H_1, \cdots, H_m, \Delta t)$, and $p_k = (4 - 4^{1/(2k-1)})^{-1}$, we have that

$$\left\| e^{-i \sum_{j=1}^m H_j \Delta t} - S_{2k}(H_1, \ldots, H_m, \Delta t) \right\| = O(|\Delta t|^{2k+1}). \tag{27}$$

Assuming again that $\|H_1\| \geq \|H_2\| \geq \cdots \geq \|H_m\|$ we normalize the Hamiltonians by setting $\mathcal{H}_j = H_j/\|H_1\|$, $j = 1, \ldots, m$, and consider the equivalent simulation problem

$$e^{-i \sum_{j=1}^{m} \mathcal{H}_j \tau},$$

where $\tau = \|H_1\|t$. Proceeding in a way similar to that for $m = 2$ of the previous section we derive the following lemma, whose proof can be found in the Appendix.

Lemma 2 *For $k \in \mathbb{N}$, $d_k|\Delta t| \leq k+1$, $d_k = m(4/3)k(5/3)^{k-1}$, $m \geq 2$, and $\|\mathcal{H}_m\| \leq \cdots \leq \|\mathcal{H}_2\| \leq \|\mathcal{H}_1\| = 1$ we have*

$$\|\exp(-i\sum_{j=1}^{m} \mathcal{H}_j \Delta t) - S_{2k}(\mathcal{H}_1, \ldots, \mathcal{H}_m, \Delta t)\| \leq \frac{4\|\mathcal{H}_2\|}{(2k+1)!}(d_k|\Delta t|)^{2k+1}. \tag{28}$$

From Lemma 2, we have the following theorem.

Theorem 2 *Let $1 \geq \varepsilon > 0$ be such that $4emt\|H_2\| \geq \varepsilon$, $m \geq 2$. The number N of exponentials for the simulation of $e^{-i(H_1+\cdots+H_m)t}$ with accuracy ε is bounded by*

$$N \leq (2m-1)\, 5^{k-1} \left\lceil \|H_1\|t \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{4me}{3}\left(\frac{5}{3}\right)^{k-1} \right\rceil,$$

for any $k \in \mathbb{N}$, where $\|H_m\| \leq \cdots \leq \|H_2\| \leq \|H_1\|$.

Proof The proof is similar to that of Theorem 1. Let $M = |\Delta t|^{-1}$. Then using Lemma 2 and $\mathcal{H}_j = H_j/\|H_1\|$, $j = 1, \ldots, m$, we obtain

$$\begin{aligned} &\left\|e^{-i(H_1+\cdots+H_m)t} - S_{2k}^{M\|H_1\|t}(\mathcal{H}_1, \ldots, \mathcal{H}_m, 1/M)\right\| \\ \leq &M\|H_1\|t \frac{4}{(2k+1)!}\|\mathcal{H}_2\| \left(\frac{d_k}{M}\right)^{2k+1} \\ = &4t\|H_2\| \frac{d_k^{2k+1}}{(2k+1)!} \frac{1}{M^{2k}}. \end{aligned} \tag{29}$$

Recall that d_k is defined in Lemma 2. For accuracy ε we obtain

$$M \geq \left(\frac{4t\|H_2\|d_k^{2k+1}}{\varepsilon(2k+1)!}\right)^{1/(2k)}.$$

We use the estimate (24). It is easy to check that

$$d_k^{1/(2k)} \leq 2m^{1/(2k)}.$$

Thus it suffices to take

$$M \geq \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{2e\, d_k}{2k+1}.$$

So we define M to be the lower bound of the expression above, i.e.,

$$M := \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{2e\, d_k}{2k+1}.$$

As in the proof of Theorem 1, it is straightforward to verify that $M(k+1) \geq d_k$. Therefore, the assumptions of Lemma 2 are satisfied for this value of M.

From the recurrence relation, we see that the number of required exponentials to implement S_{2k} in one subinterval is no more than $(2m-1) \cdot 5^{k-1}$. Again we distinguish two cases for $M\|H_1\|t$. We deal with the case $M\|H_1\|t < 1$ in the same way we did in the proof of Theorem 1, to conclude

$$N \leq (2m-1) \cdot 5^{k-1}.$$

If $M\|H_1\|t \geq 1$, then the total number of required exponentials is

$$N \leq (2m-1) \cdot 5^{k-1} \lceil M\|H_1\|t \rceil.$$

Substituting the values of M and d_k we obtain

$$N \leq (2m-1) \cdot 5^{k-1} \left\lceil \|H_1\|t \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{4me}{3} \left(\frac{5}{3}\right)^{k-1} \right\rceil.$$

This completes the proof. $\square$

The reader may wish to recall Remark 1 that applies in the case too.

Corollary 1 *If in addition to the assumptions of Theorem 2 either of the following two conditions holds:*

- $4emt\|H_1\| \geq 3$
- ε *is sufficiently small such that*

$$\left(\ln \frac{4emt\|H_1\|}{5}\right)^2 - 2\ln\frac{5}{3}\ln\frac{4emt\|H_2\|}{\varepsilon} < 0$$

then the number of exponentials, N, for the simulation of $e^{-i(H_1+\cdots+H_m)t}$ with accuracy ε is bounded by

$$N \leq 2\,(2m-1)\,5^{k-1}\|H_1\|t \left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)} \frac{4me}{3}\left(\frac{5}{3}\right)^{k-1},$$

for any $k \in \mathbb{N}$.

Proof From the assumption of Theorem 2 we have $4emt\|H_2\|/\varepsilon \geq 1$. Consider the argument of the ceiling function in the bound of Theorem 2. It is greater than or equal to 1, if $4emt\|H_1\| \geq 3$. Otherwise, we take its logarithm and multiply the resulting expression by k. This gives the quadratic polynomial

$$2k^2 \ln\frac{5}{3} + 2k\ln\frac{4emt\|H_1\|}{5} + \ln\frac{4emt\|H_2\|}{\varepsilon}.$$

When ε is sufficiently small and the discriminant is negative, i.e., when

$$\left(\ln \frac{4emt\|H_1\|}{5}\right)^2 - 2\ln\frac{5}{3}\ln\frac{4emt\|H_2\|}{\varepsilon} < 0,$$

the polynomial is positive for all k. Hence, that argument of the ceiling function in the bound of Theorem 2 is greater than 1, for all $k \geq 1$.

In either case, we use $\lceil x \rceil \leq 2x$, for $x \geq 1$, to estimate N from above. $\square$

5 Speedup

Let us now deal with the cost for simulating the evolution $e^{-i(\sum_{j=1}^{m} H_j)t}$. Berry et al. [5] show upper bounds for the number of required exponentials. We improve their estimates.

We are interested in the number of exponentials required by the splitting formula that approximates the evolution with accuracy ε. Recall that

$$N_{\rm new} := 2\,(2m-1)\,5^{k-1}\|H_1\|t\left(\frac{4emt\|H_2\|}{\varepsilon}\right)^{1/(2k)}\frac{4me}{3}\left(\frac{5}{3}\right)^{k-1} \tag{30}$$

exponentials suffice for error ε. The above estimate holds for ε sufficiently small as Theorem 2 and Corollary 1 indicate. The corresponding previously known estimate [5] is

$$N_{\rm prev} = m\;5^{2k}\;(m\|H_1\|t)^{1+\frac{1}{2k}}\left(\frac{1}{\epsilon}\right)^{\frac{1}{2k}},$$

where $H = \sum_{j=1}^{l} H_j$.

The ratio of the two estimates is

$$\frac{N_{\rm new}}{N_{\rm prev}} \le \frac{2}{3^k}\left(\frac{4e\|H_2\|}{\|H_1\|}\right)^{1/2k}. \tag{31}$$

Thus, if $\|H_2\| \ll \|H_1\|$ we have an improvement in the estimate of the cost the algorithm for all k. This is particularly significant when k is small. For instance, $k=1$ for the Strang splitting S_2, which is frequently used in the literature.

Let us now consider the optimal k, i.e., the one minimizing $N_{\rm new}$, for a given accuracy ε. It is obtained from the solution of the equation

$$2k^2\ln\frac{25}{3} - \ln\frac{4emt\|H_2\|}{\varepsilon} = 0.$$

Since we seek a positive integer $k^*_{\rm new}$ minimizing $N_{\rm new}$, we set

$$k^*_{\rm new} := \max\left\{\mathrm{round}\left(\sqrt{\frac{1}{2}\log_{25/3}\frac{4emt\|H_2\|}{\varepsilon}}\right), 1\right\},$$

where $\mathrm{round}(x) = \lfloor x + 1/2\rfloor$, $x \ge 0$. We can avoid using the max function in the expression above by considering $\varepsilon \le mt\|H_2\|$. Then the number of exponentials $N_{\rm new}$ satisfies

$$N^*_{\rm new} \le \frac{8}{3}\,(2m-1)\,emt\,\|H_1\|\;e^{2\sqrt{\frac{1}{2}\ln\frac{25}{3}\ln\frac{4emt\|H_2\|}{\varepsilon}}}.$$

Berry et al. [5] find

$$k^*_{\rm prev} = \mathrm{round}\;\left(\frac{1}{2}\sqrt{\log_5\frac{m\|H_1\|t}{\varepsilon}+1}\right), \tag{32}$$

which minimizes $N_{\rm pre}$. For $k^*_{\rm prev}$ the number of exponentials $N_{\rm prev}$ becomes

$$N^*_{\rm prev} = 2m^2\|H_1\|t\;e^{2\sqrt{\ln 5\ln\frac{m\|H_1\|t}{\varepsilon}}}. \tag{33}$$

As a final comparison with N_{prev} we have

$$\frac{N^*_{\mathrm{new}}}{N^*_{\mathrm{prev}}} \le \frac{8\,e}{3}\, e^{2\left(\sqrt{\frac{1}{2}\ln\frac{25}{3}\ln\frac{4emt\|H_2\|}{\varepsilon}}-\sqrt{\ln 5\ln\frac{m\|H_1\|t}{\varepsilon}}\right)}.$$

Hence, there is an important difference between the previously derived optimal k and the one derived in the present paper. In [5], the optimal k depends on $\|H_1\|$. More precisely, we show that the optimal k depends on $\|H_2\|$, the second largest norm of the Hamiltonians comprising H, which can be considerably smaller than $\|H_1\|$.

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7 Appendix

Proof (Proof of Lemma 2) Unwinding the recurrence for S_{2k} we see that

$$\begin{aligned} S_{2k}(\mathcal{H}_1,\dots,\mathcal{H}_m,\Delta t) &= \prod_{\ell=1}^{K} S_2((\mathcal{H}_1,\dots,\mathcal{H}_m,z_\ell\Delta t) \\ &= \prod_{\ell=1}^{K}\left[\prod_{j=1}^{m} e^{-i\mathcal{H}_j z_\ell \Delta t/2}\prod_{j=m}^{1} e^{-i\mathcal{H}_j z_\ell \Delta t/2}\right], \end{aligned}$$

where $K = 5^{k-1}$ and each z_ℓ is defined according to the recursive scheme, $\ell = 1,\dots,K$. For the details, see the part of the text that follows (4). The bound (5), namely,

$$|z_\ell| \le \frac{4k}{3^k} \qquad \text{for all } \ell = 1,\dots,K,$$

holds independently of m, because it depends on the $k-1$st levels of the recursion tree and not on the leaf, $S_2((\mathcal{H}_1,\dots,\mathcal{H}_m,z_\ell\Delta t)$, at which, the corresponding to ℓ, path ends.

In the expression of $S_2((\mathcal{H}_1,\dots,\mathcal{H}_m,z_\ell\Delta t)$ the sum of the magnitudes of the factors multiplying the Hamiltonians in the exponents is $m|z_\ell|\cdot|\Delta t|$, for all $\ell = 1,\dots,K$. Thus in the expression of S_{2k} above, the sum of the magnitudes of all factors multiplying the Hamiltonians in the exponents is

$$\sum_{\ell=1}^{K}(m|z_\ell|\cdot|\Delta t|) \le 5^{k-1} m\frac{4k}{3^k}|\Delta t|.$$

Define

$$d_k := m\frac{4}{3}k\left(\frac{5}{3}\right)^{k-1} \qquad k \ge 1. \tag{34}$$

Equivalently, one can view the expression for S_{2k} above as a product of exponentials of the form $e^{\mathcal{H}_j r_{j,n}\Delta t}$, where $\sum_{n=1}^{N_j} r_{j,n} = 1$, $j = 1,\cdots,m$, and N_j is the number of occurrences of $\mathcal{H}_j$ in S_{2k}. Recall that for $m = 2$ we used s_n to denote $r_{1,n}$ and z_n to denote $r_{2,n}$. With this notation and using (34) we have

$$\sum_{j,n} |r_{j,n}| \le d_k. \tag{35}$$

(Recall the derivation of (7).)

Expanding the factors of S_{2k} in a power series individually, and then carrying out the multiplications amongst them, we conclude that S_{2k} is given by an infinite sum whose terms have the form

$$\prod_{(j,n)} \frac{1}{\gamma_{j,n}!} \mathcal{H}_j^{\gamma_{j,n}} \left[-i\, r_{j,n}\, \Delta t\right]^{\gamma_{j,n}}. \tag{36}$$

The factors of these products are specified by the Hamiltonians H_j and the order of their occurrences after unwinding the recurrence for S_{2k}, where $j = 1, \dots, m$ and $\gamma_{j,n} = 0, 1, 2, \dots,$ for all $n = 1, \dots, N_j$.

Consider the terms that contain only $\mathcal{H}_1$ and, therefore, have $\gamma_{j,n} = 0$, for $n = 1, \dots, N_j$ and $j = 2, \dots, m$. The sum of these terms is

$$\begin{aligned}
&\sum_{\gamma_{j,n}=0 \text{ for } j\neq 1} \prod_{(j,n)} \frac{1}{\gamma_{j,n}!} \mathcal{H}_j^{\gamma_{j,n}} \left[-i\, r_{j,n}\, \Delta t\right]^{\gamma_{j,n}} \\
&= \sum_{\gamma_{1,1}=\cdots=\gamma_{1,N_1}=0}^{\infty} \prod_{(1,n)} \frac{1}{\gamma_{1,n}!} \mathcal{H}_1^{\gamma_{1,n}} \left[-i\, r_{1,n}\, \Delta t\right]^{\gamma_{1,n}} \\
&= \prod_{n=1}^{N_1} \sum_{\gamma_{1,n}} \frac{1}{\gamma_{1,n}!} H_1^{\gamma_{1,n}} \left[-i r_{1,n}\, \Delta t\right]^{\gamma_{1,n}} = \prod_{n=1}^{N_1} e^{-i\mathcal{H}_1 r_{1,n} \Delta t} \\
&= e^{-i \sum_n r_{1,n} H_1 \Delta t} = e^{-i\mathcal{H}_1 \Delta t}.
\end{aligned} \tag{37}$$

On the other hand,

$$e^{-i\sum_{j=1}^m \mathcal{H}_j \Delta t} = I + \left(-i \sum_{j=1}^m \mathcal{H}_j \Delta t\right) + \cdots + \frac{1}{k!}\left(-i \sum_{j=1}^m \mathcal{H}_j \Delta t\right)^k + \cdots, \tag{38}$$

and the terms that contain only $\mathcal{H}_1$ have sum

$$\sum_{k=0}^{\infty} \frac{1}{k!} \mathcal{H}_1^k (-i\Delta t)^k = e^{-i\mathcal{H}_1 \Delta t}. \tag{39}$$

Let us now consider the error bound in (27). The sum of the terms with only $\mathcal{H}_1$ in S_{2k+1} and $\exp(\sum_{j=1}^m H_j \Delta t)$ is the same and cancels out when we subtract one from the other. Moreover, in $\exp(-i\sum_{j=1}^m \mathcal{H}_j \Delta t) - S_{2k}(\Delta t)$ we know that the terms of order up to $2k$ also cancel out, see Eq. (27). From this we conclude that the error is proportional to $\|\mathcal{H}_2\| |\Delta t|^{2k+1}$.

Consider

$$\exp(-i(\mathcal{H}_1 + \cdots + \mathcal{H}_m)\Delta t) - S_{2k}(\mathcal{H}_1, \dots, \mathcal{H}_m, \Delta t) = \sum_{l=2k+1}^{\infty} \left[R_l(\Delta t) - T_l(\Delta t)\right], \tag{40}$$

where $R_l(\Delta t)$ is the sum of all terms in $\exp(-i(\mathcal{H}_1+\cdots+\mathcal{H}_m)\Delta t)$ corresponding to Δt^l and $T_l(\Delta t)$ is the sum of all terms in S_{2k} corresponding to Δt^l. We can ignore the terms in $T_l(\Delta t)$ and $R_l(\Delta t)$ that contain only $\mathcal{H}_1$ (and not $\mathcal{H}_2$) as a factor.

Then

$$\|R_l(\Delta t)\| = \left\| \frac{1}{l!}\left(\sum_{j=1}^{m} \mathcal{H}_j \Delta t\right)^l - \frac{1}{l!}\mathcal{H}_1^l \Delta t^l \right\| \leq \frac{m^l}{l!}\|\mathcal{H}_2\||\Delta t|^l, \tag{41}$$

because there are $m^l - 1$ terms in R_l and each norm is at most $\frac{1}{l!}\|\mathcal{H}_2\||\Delta t|^l$.

From (36) we have

$$T_l(\Delta t) = \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{(j,n)} r_{j,n}^{\gamma_{j,n}}}{\prod_{(j,n)} \gamma_{j,n}!} \prod_{(j,n)} \mathcal{H}_j^{\gamma_{j,n}} \Delta t^l, \tag{42}$$

where $\sum_n \gamma_{1,n} \neq l$, i.e., there is no terms containing only $\mathcal{H}_1$. So, $\| \prod_{(j,n)} \mathcal{H}_j^{\gamma_{j,n}} \| \leq \|\mathcal{H}_2\|$, and

$$\|T_l(\Delta t)\| \leq \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{j,n} |r_{j,n}|^{\gamma_{j,n}}}{\prod_{j,n} \gamma_{j,n}!} \|\mathcal{H}_2\||\Delta t|^l. \tag{43}$$

To calculate the coefficients of the sum, we consider

$$\begin{aligned}\prod_{(j,n)} \exp(|r_{j,n}\Delta t|) &= \prod_{(j,n)} \sum_{\gamma_{j,n}=0}^{\infty} \frac{1}{\gamma_{j,n}!}|r_{j,n}\Delta t|^{\gamma_{j,n}} \\ &= \sum_{l=0}^{\infty} \sum_{\sum \gamma_{j,n}=l} \frac{\prod_{j,n} |r_{j,n}|^{\gamma_{j,n}}}{\prod_{j,n} \gamma_{j,n}!}|\Delta t|^l.\end{aligned} \tag{44}$$

Hence the coefficient of $|\Delta t|^l$ in (43) is equal to that in (44). Also

$$\prod_{j,n} \exp(|r_{j,n}\Delta t|) = \exp(\sum_{j,n} |r_{j,n}\Delta t|). \tag{45}$$

From (35) we obtain

$$\|T_l(\Delta t)\| = \frac{d_k^l}{l!}\|\mathcal{H}_2\||\Delta t|^l. \tag{46}$$

Therefore,

$$\begin{aligned}\| \exp(\sum_{j=1}^{m} \mathcal{H}_j \Delta t) - S_{2k}(\Delta t)\| &\leq \sum_{l=2k+1}^{\infty} \|R_l(\Delta t)\| + \|T_l(\Delta t)\| \\ &\leq 2 \sum_{l=2k+1}^{\infty} \frac{d_k^l}{l!}\|\mathcal{H}_2\||\Delta t|^l \\ &= 2\|\mathcal{H}_2\| \sum_{l=2k+1}^{\infty} \frac{1}{l!}|d_k \Delta t|^l \\ &\leq \frac{2}{(2k+1)!}\|\mathcal{H}_2\||d_k\Delta t|^{2k+1}\left(1 - \frac{d_k|\Delta t|}{2k+2}\right)^{-1} \\ &\leq \frac{4}{(2k+1)!}\|\mathcal{H}_2\||d_k\Delta t|^{2k+1},\end{aligned} \tag{47}$$

where the last two inequalities follow from the assumption $d_k|\Delta t| \leq k+1$ and an estimate of the tail of the Poisson distribution; see, e.g., [16, Thm 1]. □

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