Quantum simulation promises to address many challenges in fields ranging from quantum chemistry to material science and high-energy physics, and could be implemented in noisy intermediate scale quantum devices. A challenge in building good quantum digital simulators is the fidelity of the engineered dynamics, which stems from practical experimental constraints. While the approximation in building the target Hamiltonian by a Trotter construction could be improved by taking smaller steps, this is not always possible experimentally. Here we provide an alternative construction, which we call Quantum Interpolation, that locally minimizes the error and achieves better fidelity than the Trotter expansion for the same minimum time step and time-step resolution. Our Quantum Interpolation construction can be found from a simple geometric condition, thus is computationally efficient. Thanks to its improved fidelity, Quantum Interpolation can form the basis for experimental-constrained quantum digital simulation.

I. INTRODUCTION

Simulation has been at the core of quantum information processing right from its inception, starting from Feynman’s vision of simulating physics using a quantum system [1]. Quantum simulators are posed to be one of the first quantum devices to show task-specific quantum supremacy [2]. Quantum simulation has great potential impact on quantum chemistry [3–5], material science [6], condensed matter [7–10], and high-energy physics [11, 12]. The most flexible strategy to achieve quantum simulation is via digital quantum simulation [13], where a target time-evolution operator is represented by a sequence of elementary quantum gates, usually involving one or two qubits. This type of constructions, where the desired dynamics is obtained from evolution under piecewise constant Hamiltonians, has broader applicability than digital quantum simulation. For example, it is at the core of pulse dynamical decoupling [14, 15] and coherent averaging in NMR [16], it is used to achieve time-optimal bang-bang control [17–19], and it has also been recently applied to solving optimization problems that are classically difficult [20]. Digital quantum simulation finds broad application on various platforms due to its flexibility, including superconducting qubits [8, 9, 21, 22], trapped ions [7, 23], atomic systems [24], and spin systems [10, 25, 26].

The backbone of digital quantum simulation is the Trotter expansion [27], which is used to build the simulated Hamiltonian from elementary blocks. Thus, finding a sequence of elementary operations that gives the desired simulated Hamiltonian with high fidelity is crucial to digital quantum simulation. In all experimental systems, the smallest step in the Trotter expansion is bound by experimental constraints, such as finite length of control pulses and finite clock rate, thus limiting the expansion fidelity. For example, in a recent implementation of digital quantum simulation with trapped ions [7], the smallest flip angle of the unitary evolution block was $Jt = \pi/16$, and similar numbers can be obtained in other experimental platforms. Then, even the second order Trotter construction might not yield good enough fidelity, while higher order expansions are usually hard to implement experimentally with the desired precision due to the complex, sometimes negative [28] and even imaginary [29], coefficients.

Another experimental constraint might also be given by the minimum time resolution with which one can vary the Trotter time step. Conversely, it is often required to finely vary the parameters of the effective, simulated Hamiltonian, in order to study e.g. the dynamics across (dynamical) quantum phase transitions [25, 30, 31], such as due to localization [10, 32, 33]. Depending on experimental platforms, the shortest evolution time and the time-step resolution may not always be the same. In this paper we mainly take them as the same and also provide discussion on the case where in second order Trotter expansion the time-step resolution in relaxed.

As the fidelity of the Trotter expansion might change when varying the target Hamiltonian to be engineered from the same building blocks, this might obscure the experimental results. It thus becomes imperative to find alternative expansions that might not suffer from this problem.

Motivated by these realistic experimental limitations – the shortest evolution time, time-step resolution, and implementable Hamiltonians – we present a novel construction, that we call Quantum Interpolation (QI), to approximate an average exponential operator. QI is a second order expansion in the minimum step size or time-step resolution, but it achieves a higher fidelity (and more robust performance with respect to the target Hamilto-
nian) when compared to second order Trotter expansion. This is particularly important since often the minimum step and time-step resolution are fixed. We further compare our construction with the Trotter expansion in terms of the number of operations required to switch from one Hamiltonian block to the next, which could introduce additional errors; we find that even considering this added cost, there are regimes where QI is beneficial. We also compare QI with second order Trotter where the time-step resolution is not limited for second order Trotter expansion.

The paper is organized as follows. We first introduce the Quantum Interpolation construction and provide a simple geometric interpretation to explain the algorithm used to find the construction. We then analyze both analytically and numerically the performance of QI, with respect to the most relevant parameters. Before concluding, we show how to extend QI to quantum simulations requiring to combine more than two basic blocks.

II. QUANTUM INTERPOLATION CONSTRUCTION

We consider the problem of engineering a target operator \( e^{pA+qB} \), which encapsulates a general quantum simulation task, using evolution under the operators \( A \) and \( B \). Here we assume \( p \) and \( q \) to be integers and mutually prime and that we are limited by experimental constraints on the shortest evolution time and time-step resolution to only construct \( e^{A/n} \) and \( e^{B/n} \) (where \( n > 0 \) is also an integer). The most straightforward approach is to use the first order Trotter expansion as a guide for the quantum simulation protocol, \( (e^{pA/n}e^{qB/n})^n \approx e^{pA+qB} \).

If \( p \) (or \( q \)) is even, we can follow the second order Trotter expansion,

\[
\left( e^{pA/(2n)} e^{qB/n} e^{pA/(2n)} \right)^n \approx e^{pA+qB}
\]

(and similarly for \( q \) even) to achieve a better approximation. Higher order Trotter expansions have the general form of \( e^{pA+qB} \approx e^{c_1pA} e^{c_2qB} e^{c_3pA} \cdots e^{c_mpB} \), where however the coefficients \( pc_1,3,\ldots \) and \( qc_2,4,\ldots \) are usually not integers and can even be negative and thus typically challenging (or impossible) to implement experimentally. One example of third order Trotter expansion is Ruth’s formula [34],

\[
\left( e^{pA} e^{qB} e^{pA} e^{-qB} e^{pA} e^{qB} \right)^n \approx e^{pA+qB},
\]

where negative coefficients are used. Indeed, some negative coefficients are unavoidable in third and higher order Trotter expansions [28]. Implementing "time reversal" to construct the unitaries with negative coefficients is not always possible.

Here we present Quantum Interpolation, a new second order exponential product approximation, which can be practically implemented in experiments and has better fidelity than the second order Trotter expansion. We can generally write the QI expansion as

\[
\left( e^{pa_1A/n} e^{qb_1B/n} \cdots e^{pa_MA/n} e^{qb_MB/n} \right)^n \approx e^{pA+qB},
\]

where \( \sum_{k=1}^M a_k = \sum_{k=1}^M b_k = 1 \) and \( pa_k, qb_k \) are integers \( \forall k \).

Quantum Interpolation offers an algorithm to obtain an ordering of \( e^{A/n} \) and \( e^{B/n} \) (by setting the coefficients \( a_k, b_k \)), which locally minimizes the error. In the usual Trotter expansion based on \( e^{A/n} e^{B/n} \), the \( e^{A/n} \) and \( e^{B/n} \) operators are clustered together in \( p \) and \( q \) groups. Quantum Interpolation enables taking advantage of the smallest unitary step experimentally accessible, \( e^{A/n} \) and \( e^{B/n} \); intuitively, spreading out these two basic blocks as much as possible generates additional higher order terms in the Trotter expansion. By selecting a locally optimal ordering, these higher orders provide a better approximation to the desired operator \( e^{pA+qB} \).

In other words, QI offers a finer ordering of \( e^{\pi} \) and \( e^{\hat{X}} \) and thus a higher digital resolution [38], which reduces the error in the exponential approximation.

A geometric interpretation of the algorithm used to find the QI construction is shown in Fig. 1(A). The ideal

FIG. 1. Quantum Interpolation construction. (A) Geometric explanation of the intuition of Quantum Interpolation. (B) Quantum Interpolation...
operator $e^{pA+qB}$ can be represented as a vector $(p, q)$. Starting from the origin $(0, 0)$, at each step we can move up (evolving under $e^B$) or right (evolving under $e^A$). The strategy is to choose at each step the move which ends closer to the diagonal. This in turns optimizes the propagator fidelity at each step. The area enclosed between the path and the diagonal qualitatively represents error. Fig. 1(B) shows the ordering of $e^A$ (red) and $e^B$ (white) for all possible $p + q = 24$. This geometric picture can be easily generalized to higher dimension (see Fig. 6(B)), that is, to combine a larger number of propagators, $e^{A/n}, e^{B/n}, e^{C/n}, \ldots$.

QI is a greedy algorithm as it minimizes the error at each step. This simplifies tremendously the optimization, as it does not even require calculating the quantum mechanical propagators, which might be prohibitive when considering large quantum systems for quantum simulation. While we do not attempt to find a global optimum, we can perform a simple step in that direction, by symmetrizing the construction. For example, if the ordering is not already symmetric, by repeating the sequence in reverse order we create a palindromic ordering that ensures that the the first order correction (and odd higher orders) are canceled, that is, QI can be made into a second order expansion by symmetrization.

III. PERFORMANCE OF QUANTUM INTERPOLATION

A. Analytical bounds on fidelity

We can prove that Quantum Interpolation provides a better second-order approximation to the desired operator. The details of the proof can be found in Appendix A; here we only state the main idea. To achieve a target evolution $e^{pA+qB}$, the second order Trotter expansion can be written in two forms: $e^{\frac{p}{2}A}e^{B}e^{\frac{q}{2}A}$ or $e^{\frac{q}{2}B}e^{A}e^{\frac{p}{2}B}$. The approximation error is different, unless $p = q$ and $[A, [A, B]] = [B, [A, B]]$. The proof demonstrates that Quantum Interpolation provides better performance than the best of the two Trotter expansions. The proof has two steps. In the first step we show that any construction of the type in Eq. (3), when appropriately symmetrized as discussed above, has an error that is bounded by the worst case of the two Trotter forms. The second step shows that Quantum Interpolation further excludes any construction with error larger than the best Trotter expansion, by appropriately choosing the ordering of the timings in Eq. (3). Thus the error of Quantum Interpolation is always bounded by the better case of the two second-order Trotter expansions.

B. Fidelity

To support our analytical results, we tested the performance of Quantum Interpolation numerically on a few spin models. The metric we use to quantify the performance is the average fidelity of a quantum gate [39], which reads

$$F = \frac{\text{Tr}(U_i^1U_2)}{\text{Tr}(U_i^1)}$$

where $U_1$ is the ideal operator and $U_2$ is the approximated one. To further highlight differences in fidelity, we typically plot the log-fidelity $F_l = -\log(1 - F)$.

Fig. 2 shows typical results for a two-spin transverse-field Ising Hamiltonian, $H = pH_1 + qH_2$, where $H_1 = \frac{1}{2}(\sigma_z^1 + \sigma_z^2)$ and $H_2 = \sigma_x^1\sigma_x^2$. Then $A = -iH_1$, $B = -iH_2$, and $x = \frac{s}{n}$ is the smallest evolution step as well as the time-step resolution. We can show that for most pairs $(p, q)$ (here with $p + q = 10$) QI provides a higher fidelity than second order and even third order Trotter expansion [see Fig. 2(A)]. Note that at $(2, 8), (8, 2)$, and $(5, 5)$, the second order Trotter expansion and Quantum Interpolation share the same construction thus they give the same fidelity. Averaging over all possible $(p, q)$ pairs with $p + q = 100$, Quantum Interpolation has a much...
better performance than other decompositions for all $n$ [Fig. 2(B)].

We can further verify that QI is a second order expansion with respect to $x = t/n$, as shown analytically in Appendix A. Here we show numerically with one example $p = 6, q = 7$. In Fig. 2(C) we show the slopes of first order Trotter, second order Trotter, Quantum Interpolation, and Ruth’s formula have a ratio $2:3:3:4$, which shows that the leading order of error is proportional to $t^3$ and Quantum Interpolation is indeed a second order expansion.

We can also verify that the same qualitative results apply for different Hamiltonians (e.g., for single particle operators, for larger transverse-field Ising models, with $N = 2 - 10$ spins, etc.)

While the comparison to well-known Trotter decomposition is instructive, one might think that simple alternative constructions could be found heuristically. For example, the intuition behind Quantum Interpolation is to maximize the alternation (spreading out) of the two operators, $e^{A/n}$ and $e^{B/n}$. For many $(p, q)$ pairs, however, it is not simple to find an exact alternating ordering. Then, a naive alternation construction is still outperformed by QI, see e.g., Fig. 3 for several examples.

**C. Number of switches**

While QI reaches better fidelity than the Trotter expansion, it generally does so by increasing the number of alternations between the two (or more) building blocks $A$ and $B$. In many experimental implementations, switching between the two Hamiltonians comes at a cost, either because of additional time overheads, or because the switch itself, obtained e.g., by applying a short control pulse, might introduce control errors. Still, large number of pulses have routinely been applied e.g., in dynamical decoupling [36, 40] and Hamiltonian engineering [10], so a large number of switches is not infeasible. Quantifying the decrease in fidelity due to such errors is complex, because it would be platform dependent. Still, we can evaluate the number of switchings required to achieve a certain fidelity for different constructions. We find that QI does not always impose an overhead in the number

**FIG. 3. Comparison with naive alternation.** We compare the fidelity of QI with constructions naively obtained by alternating as much as possible the two basic operators, $e^A$ and $e^B$. The fidelity as a function of the smallest step $t$ is better for QI than for the naive constructions. We consider three cases, all with $p + q = 32$ and $p = 6, 13$ and $15$, and we set $n = 100$. The QI and naive constructions are pictorially depicted with white boxes indicating $e^B$ and red (blue) boxes $e^A$ for the QI (naive) construction.

**FIG. 4. Number of switches.** $t = 1, p + q = 10$. This figure shows the total number of operations (switches) needed to reach a certain fidelity.

**FIG. 5. Comparison between QI and second order Trotter with infinitely high time resolution.** The four region a, b, c, and d correspond to $p \geq 2q$, $q \leq p < 2q$, $q/2 \leq p < q$, and $p < q/2$ respectively, where the best Trotter expansion differ. In this calculation, $H_1 = \frac{1}{2}(\sigma_1^x + \sigma_2^x)$ and $H_2 = \sigma_1^z\sigma_2^z$ are used. $p + q$ is fixed at 100, $t = 1$ and $n = 20$. We choose a number of Trotter steps, $n = 20$, that is in the range of what used in digital quantum simulation with superconducting qubits [8] (where $J \sim 40$MHz, $\Delta t \sim 1$ns and $1/n = J\Delta t = 1/25$) and in the manipulation of relatively strongly coupled nuclear spins with Nitrogen Vacancy center in diamond [36].
FIG. 6. QI for three operators. (A) $t = 1$, $n = 10$, $p + q + r = 12$. (B) The trajectory of QI for two examples (3,4,5) and (6,4,2).

D. Performance when the time-step resolution is not limited

Quantum Interpolation outperforms second order Trotter under constraints on both the smallest evolution time as well as the time-step resolution (that is, the duration of each time step cannot be set at will, as long as it is above the smallest time step, but it can only increase by a finite amount). Fast qubits suffer from these two limitations in real experiments, since typically the timing of each operation is set by a digital clock with a minimum resolution. However, for qubits that present a slow dynamics, such constraints are very weak to nonexistent. In these cases, assuming that there are no constraints on time resolution, second order Trotter typically performs better than QI that by construction assumes a finite time-step resolution (equal to the minimum time step). In Fig. 5 we compare the second order Trotter and QI constructions for different $p, q$. Note that for different $p, q$ values, there is an optimal second order Trotter expansion, which is the one we selected. Still, we see that QI has better performance than second order Trotter for certain $p, q$ values.

IV. EXTENSION TO THREE OPERATORS

Using the geometric picture, Quantum Interpolation can be easily extended to three or more operators. The greedy algorithm always find the step that keeps the trajectory closest to the diagonal. Here we tested the performance of quantum Interpolation on a two-qubit Ising Hamiltonian with both transverse and longitudinal fields. The three implementable Hamiltonians read

$$H_1 = \sigma_z^1 \sigma_z^2, \quad H_2 = \frac{1}{2} (\sigma_z^1 + \sigma_z^2), \quad H_3 = \frac{1}{2} (\sigma_x^1 + \sigma_x^2)$$

and the target evolution is $e^{-i(pH_1 + qH_2 + rH_3)t}$, where $p, q, r$ are integers with greatest common divisor 1.

We compare in Fig. 6 the results for QI and the first-order Trotter expansion (for simplicity, we did not symmetrize either QI or Trotter, so that both are now first-order approximation constructions). We see that QI outperforms the Trotter expansion even in this more complex construction. Similar results can be obtained with different Hamiltonians.

V. CONCLUSIONS

We presented a novel construction to achieve better fidelity in quantum digital simulation. By finding a locally optimal ordering of the simulation building block, Quantum Interpolation improves the evolution fidelity with respect to the widely used second-order Trotter expansion. Our construction would be useful in the presence of experimental limitations on the minimum step and time-step resolution that one can evolve under each basic Hamiltonian. We further evaluated its performance with respect not only to the time step, but also to the number of “switching” operations needed, finding that Quantum Interpolation performs well even under this metric. We also made comparisons between Quantum Interpolation and second order Trotter where the time-step resolution is not limited for second order Trotter and found that the performance of Quantum Interpolation is still comparable to second order Trotter even though this condition is in favor of second order Trotter. We note that while we mostly presented numerical results for two qubits, similar performances where also obtained numerically for larger
systems, and indeed the scalings founds are expected to apply to many-qubit systems. As the minimization algorithm is very efficient, since it does not require to evaluate quantum propagators, and it can be easily extended to deal with multiple building block operators, Quantum Interpolation can become a versatile and powerful tool to improve the fidelity of quantum digital simulation for many-qubit systems.

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Appendix A: Proof of the analytical bounds on fidelity

Assume the target evolution is $e^{x(pA+qB)}$, where $p$ and $q$ are mutually prime integers \[41\] and $x$ is a small parameter (e.g., $x = 1/n$ in the previous section).

Approximating the desired evolution with a second order Trotter expansion gives

$$e^{x^2pA}e^{xqB}e^{x^2pA} = e^{x^2(pA+qB)} + x^3\mathcal{E} + O(x^4) \quad \text{(A1)}$$

or

$$e^{x^2qB}e^{x^2pA}e^{xqB} = e^{x^2(pA+qB)} + x^3\mathcal{E} + O(x^4) \quad \text{(A2)}$$

where $\mathcal{E}$ is the error operator. For Eq. (A1) we have

$$\mathcal{E} = \frac{pq}{24}(pC + 2qD), \quad \text{(A3)}$$

and for Eq. (A2) we have

$$\mathcal{E} = -\frac{pq}{24}(2pC + qD), \quad \text{(A4)}$$

where we defined $C = [A, [A, B]]$ and $D = [B, [A, B]]$.

The symmetrized QI decomposition has a general form

$$e^{\frac{a_{M+1}}{2}xpA}e^{\frac{bk}{2}xqB} \ldots e^{\frac{a_{1}}{2}xpA}(e^{\frac{b_{1}}{2}xqB}e^{\frac{a_{1}}{2}xpA}e^{\frac{b_{2}}{2}xqB})e^{\frac{a_{2}}{2}xpA} \ldots e^{\frac{b_{M}}{2}xqB}e^{\frac{a_{M+1}}{2}xpA}, \quad \text{(A5)}$$

where $\sum_{k=1}^{M+1} a_k = \sum_{k=1}^{M} b_k = 1$, and $a_k \geq 0$, $b_k \geq 0$. We can evaluate the error by starting from the middle of the sequence and keeping track of the third order error:

$$e^{\frac{a_{1}}{2}xpA}e^{\frac{b_{1}}{2}xqB} = e^{a_1xpA + b_1xqB} + x^3\mathcal{E}_1 + O(x^4) \quad \text{(A6)}$$

The error $\mathcal{E}_1$ can be written as

$$\mathcal{E}_1 = \frac{pq}{24}a_1b_1(2p a_1C + q b_1D). \quad \text{(A7)}$$

Consider the next layer

$$e^{\frac{a_{2}}{2}xpA}(e^{a_1xpA + b_1xqB} + x^3\mathcal{E}_1) e^{\frac{a_{2}}{2}xpA}$$

$$= e^{[a_1 + a_2]xpA + b_1xqB} + x^3(\mathcal{E}_2 + \mathcal{E}_1) + O(x^4), \quad \text{(A8)}$$

where

$$\mathcal{E}_2 = -\frac{pq}{24}a_2b_1 \left[ p(a_2 + 2a_1)C + 2q b_1D \right]. \quad \text{(A9)}$$

In general, we can find the formulas for the odd/even errors:

$$\mathcal{E}_{2k-1} = \frac{pq}{24}b_kA_k \left[ 2p A_kC + q(2B_{k-1} + b_k)D \right] \quad \text{(A10)}$$

$$\mathcal{E}_{2k} = -\frac{pq}{24} a_{k+1}B_k \left[ p(a_{k+1} + 2A_k)C + 2q B_kD \right], \quad \text{(A11)}$$

where $A_k = \sum_{i=1}^{k} a_i$ and $B_k = \sum_{i=1}^{k} b_i$. We want to compare the total error, $\mathcal{E}_{\text{QI}} = \sum_{k=1}^{M} (\mathcal{E}_{2k} + \mathcal{E}_{2k-1})$ with the Trotter expansion error. We use the Frobenius norm to compare operators, $\|E\|^2 = \text{Tr}(E^\dagger E)$, and without loss of generality we assume $\|C\|_F = \|D\|_F$, and to simplify the presentation we also take $\text{Tr}(C^\dagger D) = 0$. If $\|C\|_F \neq \|D\|_F$ we can rescale $p$ to make $\|C\| = \|D\|$. Hereafter we can drop the subscript $F$ without causing confusion. With these assumptions, it is straightforward to show that $\|\mathcal{E}_{\text{QI}}\| \leq \|\mathcal{E}\|$ if $p^2C^2 + q^2D^2 \leq \min(p^2 + 4q^2, q^2 + 4p^2)$, where

$$C = \sum_{k=1}^{M} [2A_k^2b_k - a_{k+1}B_k(a_{k+1} + 2A_k)], \quad \text{(A12)}$$

$$D = \sum_{k=1}^{M} [A_kb_k(b_k + 2B_{k-1}) - 2a_{k+1}B_k^2]. \quad \text{(A13)}$$

Note that $B_{k-1}$ only exists when $k \geq 2$. Indeed, we have $\mathcal{E}_{\text{QI}} = \frac{pq}{24}(pC + qD)$. Define function $f(a_1, \ldots, a_{M+1}, b_1, \ldots, b_M) = p^2C^2 + q^2D^2$. We can show that any choice of the coefficients $a_i$, $b_i$ that does not collapses the QI expansion onto the two Trotter ones gives a lower error than $\max(\|\mathcal{E}\|, \|\mathcal{E}'\|)$. The strategy is to find the upper bound of $f$ by varying $a_i$ and $b_i$ recursively.

We can start by varying the $a_{M+1}$ parameter. First change $a_1, a_2, \ldots, a_M, a_{M+1}$ to a set of independent parameters $A_2, A_2, \ldots, A_{M-1}, a_M = 1 - a_{M+1} - A_{M-1}, A_M$. After this change $a_{M+1}$ is an independent variable. All the terms in $C$ that dependents on $a_{M+1}$ are $3b_M(1 - a_{M+1})^2 - B_M + A_{M-1}(B_M - b_M)$ therefore

\[3b_M(1 - a_{M+1})^2 - B_M + A_{M-1}(B_M - b_M)\]
\[
\frac{\partial \mathcal{C}}{\partial a_{M+1}} = -6b_M(1-a_{M+1}) \leq 0, \quad \text{and} \quad (A14)
\]
\[
\frac{\partial^2 \mathcal{C}}{\partial a_{M+1}^2} = 6b_M \geq 0. \quad \text{(A15)}
\]

\[
\mathcal{C}(a_{M+1}) \text{ is a decreasing function and } \mathcal{C}(a_{M+1} = 0) = 2,
\]
\[
\mathcal{C}(a_{M+1} = 1) = -1. \quad \text{Actually } \mathcal{C}(a_{M+1}) = 3b_M a_{M+1}^2 - 6b_M a_{M+1} + 2.
\]

Similarly we find
\[
\frac{\partial D}{\partial a_{M+1}} = 3b_M(b_M - 2B_M) \leq 0, \quad \text{and} \quad (A16)
\]
\[
\frac{\partial^2 D}{\partial a_{M+1}^2} = 0. \quad \text{(A17)}
\]

\[
D(a_{M+1}) \text{ is a decreasing function and } D(a_{M+1} = 0) = 1,
\]
\[
D(a_{M+1} = 1) = -2. \quad \text{Actually } D(a_{M+1}) = 3b_M(b_M - 2)a_{M+1} + 1.
\]

The derivatives of the function
\[
f(a_1, \ldots, a_{M+1}, b_1, \ldots, b_M) = p^2 \mathcal{C}^2 + q^2 D^2
\]
are given by
\[
\frac{\partial f}{\partial a_{M+1}} = 2p^2 \mathcal{C} \frac{\partial \mathcal{C}}{\partial a_{M+1}} + 2q^2 D \frac{\partial D}{\partial a_{M+1}}, \quad \text{and} \quad (A18)
\]
\[
\frac{\partial^2 f}{\partial a_{M+1}^2} = 2p^2 (\frac{\partial \mathcal{C}}{\partial a_{M+1}})^2 + 2p^2 \mathcal{C} \frac{\partial^2 \mathcal{C}}{\partial a_{M+1}^2}
\]
\[
+ 2q^2 (\frac{\partial D}{\partial a_{M+1}})^2 + 2q^2 D \frac{\partial^2 D}{\partial a_{M+1}^2}. \quad \text{(A19)}
\]

Plugging Eq. (A14), (A15), (A16), (A17) into (A19) we find that when \( \mathcal{C} > 0, f \) is a convex function of \( a_{M+1} \) and we have \( f \leq \max \{f(a_{M+1} = 0), f(a_{M+1} = 1)\} \). When \( \mathcal{C} \leq 0, \) it is not difficult to verify that we also have \( D \leq 0 \). Even if \( \frac{\partial^2 f}{\partial a_{M+1}^2} \leq 0 \), we still have \( \frac{\partial f}{\partial a_{M+1}} \geq 0 \) and \( f \leq \max \{f(a_{M+1} = 0), f(a_{M+1} = 1)\} \) is still true.

When \( a_{M+1} = 1 \) (that is, all other coefficients \( a_1, \ldots, a_M \) are zero, meaning that \( M = 0 \) ) \( \mathcal{C} = -1 \), \( D = -2 \) and \( f = p^2 + 4q^2 \), as expected, since we retrieve the simpler Trotter expansion \( e^{\frac{2}{p}p^2A}e^{\frac{2}{q}q^2B} \).

When \( a_{M+1} = 0 \), we can repeat the same analysis above, now taking the derivatives with respect to \( b_M \). We find again that for \( b_M = 1 \) the construction collapses to the Trotter expansion \( e^{\frac{2}{p}p^2A}e^{\frac{2}{q}q^2B} \), and we can analyze the case \( b_M = 0 \) as done above. Recursively, we thus find that \( f \leq 4p^2 + 4q^2 \), with equality in the case where the construction simplifies to the Trotter expansion \( e^{\frac{2}{p}p^2A}e^{\frac{2}{q}q^2B} \) or \( f \leq p^2 + 4q^2 \), with equality in the case where the construction simplifies to the Trotter expansion \( e^{\frac{2}{p}p^2A}e^{\frac{2}{q}q^2B} \).

When \( p = q \), this proves that any decomposition of the exponential operators with more and smaller steps than the second order Trotter expansion yields a smaller error than the Trotter expansion.

When \( p \neq q \), construction with form in Eq. (A5) has an error that is bounded by \( \max(||E||, ||E'||) \). We can further show that the error of QI is actually bounded by \( \min(||E||, ||E'||) \). When \( p > q \), \( ||E|| < ||E'|| \) and we want to show that \( f \leq p^2 + 4q^2 \). According to the construction of QI, when \( p > q \), we take first \( m \) steps along \( A \), where \( \frac{q}{p+q} < \frac{1}{2} \) and \( \frac{(m+1)q}{p+q} > \frac{1}{2} \), i.e., \( m = \lfloor \frac{p+q}{2q} \rfloor \). The construction that is closest to \( e^{\frac{2}{p}p^2A}e^{\frac{2}{q}q^2B} \) allowed by QI writes
\[
e^{\frac{2m}{p}p^2A}e^{\frac{2}{q}q^2B}e^{(1-\frac{2m}{p})p^2A}e^{\frac{2}{q}q^2B} = \frac{2m}{p}p^2A \quad \text{(A20)}
\]

For decomposition Eq. (A20), we find that \( \mathcal{C} = 3(1-\frac{2m}{p})-1 = D = 1-\frac{2m}{p} \). It’s not difficult to verify that \( p^2\mathcal{C}^2 + q^2 D < p^2 + 4q^2 \), when \( p > q \). If we further decompose the central part \( e^{\frac{2}{p}p^2A}e^{(1-\frac{2m}{p})p^2A}e^{\frac{2}{q}q^2B} \), since \( q \geq 1-\frac{2m}{p} \), the worst case will converge to \( e^{\frac{4}{p}p^2A}e^{\frac{4}{q}q^2B}e^{\frac{4}{p}p^2A} \), with which the whole formula becomes \( e^{\frac{4}{p}p^2A}e^{\frac{4}{q}q^2B}e^{\frac{4}{p}p^2A} \). In other words, however you decompose the central part in Eq. (A20), the error of the whole formula is bounded by \( p^2 + 4q^2 \). In summary, when \( p > q \), if we construct the nested structure according to the principle of QI, the error will be smaller than \( p^2 + 4q^2 \). Similarly when \( p < q \), \( f \leq q^2 + 4p^2 \). In summary \( f \leq \min(p^2 + 4q^2, q^2 + 4p^2) \) and thus \( ||\mathcal{E}_{QI}|| \leq \min(||E||, ||E'||) \).

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If that is not the case and they have a common divider $m$, we can set $p' = p/m$, $q' = q/m$ and find the construction for $U' = e^{x(p'A+q'B)}$ for $n$ and then repeat it $m$ times.