A Trotter-Suzuki approximation for Lie groups with applications to Hamiltonian simulation

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We present a product formula to approximate the exponential of a skew-Hermitian operator that is a sum of generators of a Lie algebra. The number of terms in the product depends on the structure of the operators in the Hamiltonian. When the norm of the effective operator resulting from nested commutators is less than the product of the norms, the number of terms in the product is significantly less than that obtained from well-known results. We apply our results to construct product formulas useful for the quantum simulation of some continuous-variable and bosonic physical systems, including systems whose potential is not quadratic. For many of these systems, we show that the number of terms in the product can be sublinear or even subpolynomial in the dimension of the relevant local Hilbert spaces, where such a dimension is usually determined by the energy scale of the problem. Our results emphasize the power of quantum computers for the simulation of various quantum systems.

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The simulation of quantum systems is one of the most promising applications of quantum computers [1, 2]. A main challenge to devise quantum algorithms for physics simulation is to approximate the evolution operator, \( U := e^{-iHt} \), as a sequence of simple gates. Typically, this is done by using a product formula based on the so-called Trotter-Suzuki approximation [3, 4]. When the Hamiltonian \( H \) is expressed as a sum of “simple” Hamiltonians, such a product can be interpreted as an approximation of \( U \) by short-time evolutions under each simple Hamiltonian. The complexity of the algorithm is then related to the number of terms in the product. When the Hamiltonians are bounded and time independent, this number is \( O(\exp(1/\eta)(\|H\|t)^{1+\eta}) \) in the best case, for arbitrary small \( \eta > 0 \) [5, 6]. More recently, a new method for simulating the evolution operator was introduced in [7–8]. This method approximates \( U \) by implementing a truncated Taylor series of the exponential. When the Hamiltonians are bounded and under some additional assumptions, the complexity of this method is \( \tilde{O}(\|H\|t) \). (The \( \tilde{O} \) notation hides logarithmic factors.) This complexity is almost linear in the evolution time and can be shown to be optimal, i.e., there is a matching lower bound [7]. Methods for approximating \( U \) are also useful for, e.g., simulating physical systems with Monte-Carlo and other classical methods, and for simulating differential equations with the split-step Fourier method [9].

Several works study the potential of the above methods in particular examples, such as quantum chemistry and physical systems with various particle statistics (c.f., [10–17]). However, a main inconvenience of the methods in [5–8] and other related methods (c.f., [18–20]) is that they cannot be directly applied to the case of, for example, unbounded operators, or can lead to unnecessary complexity overheads. These methods also consider the worst case scenario and do not exploit certain structures of the problem, such as commutation relations between the simple Hamiltonians. For example, consider the case \( H = J_x + J_y \), where \( J_\alpha, \alpha = x, y, z \), are the well-known \( su(2) \) angular momentum operators acting on a (spin) system of dimension \( 2J + 1 \). In this case, \( \|J_\alpha\| = O(J) \) and the results in [5–8] would yield an approximation of \( U \) as a product of a polynomially large (in \( J \) ) number of exponentials \( J_x \) and \( J_y \). However, one can exactly decompose \( U \) (up to a phase) using three exponentials by means of Euler-angle decompositions [21] or obtain a very good approximation of \( U \) with a number of exponentials that is subpolynomial in \( J \), which is a consequence of our main results described below.

In this paper, we build upon the results in [5–8] and consider the case in which the simple Hamiltonian terms belong to a certain Lie algebra. By exploiting the structure in commutation relations, our main result is a significantly improved bound on the number of terms in the product formula that approximates \( U \). We illustrate our main result with several examples. The first example regards the quantum harmonic oscillator (QHO), where the operators in the Hamiltonian generate a Lie algebra of dimension 3. For the QHO, we show that \( U \) can be approximated by a sequence of simple unitaries of length subpolynomial in the dimension of the relevant Hilbert subspace, recovering a result in [22]. The second example regards coupled QHOs and we show that the number of exponentials in the approximation of \( U \) is also subpolynomial in the dimension of the local Hilbert subspaces. The third example regards a one-dimensional quantum system where, unlike the QHO, the potential is not necessarily quadratic. Depending on the form of the potential, the number of terms in the approximation of \( U \) can be sublinear or subquadratic in the dimension of the relevant Hilbert subspace.

A common feature in all these examples is that the
norm of the effective operator resulting from nested commutators of operators in the Lie algebra can be shown to be significantly smaller than the product of the norms of all effective operators appearing in such commutators. The effective operator is basically the operator projected on a relevant and finite dimensional Hilbert subspace. In our examples, the dimension of such subspaces is typically determined by an energy scale associated with the problem. While we do not construct quantum algorithms for simulating \( U \), our results suggest that quantum computers can simulate the evolution of several continuous-variable quantum systems more efficiently than conventional computers. A step in this direction was recently given in [22], where we provided a quantum algorithm for simulating the QHO with subpolynomial complexity. Classical algorithms for these problems are expected to have a worst-case complexity that is polynomial (e.g., worse than quadratic) in the dimension of the Hilbert subspaces, as one has to deal with matrices of polynomial dimension.

Additional related work.— A detailed analysis of the approximation error induced by the so-called second order Trotter-Suzuki approximation, in terms of commutators, was recently done in [15] for the quantum chemistry problem, and subsequently analyzed in [23]. The resulting number of terms in the approximation is still scales with \( \| H \| \) for that case. In contrast, our work is more concerned with problems where the the norm of the effective operators can be large, as in the case of the quantum simulation of continuous-variable quantum systems. Our goal is to provide a product formula where the number of terms can be sublinear in the norm of the effective Hamiltonian.

We define the problem and state our main results in more detail. Some applications for the simulation of relevant quantum systems are discussed later.

Problem statement.— We let \( g \) be a real Lie algebra of infinite or finite dimension \( K \) with basis \( \{ h_1, \ldots, h_K \} \). Since we are interested in the case where \( U \) is unitary, we assume that \( h_k \) is skew-Hermitian for all \( k \). The Lie bracket is \([ h_k, h_{k'} ] := h_k h_{k'} - h_{k'} h_k \) and

\[
[h_k, h_{k'}] = \sum_{k''=0}^{K} \gamma_{k,k'}^{k''} \hat{h}_{k''} .
\]

The constants \( \gamma_{k,k'}^{k''} \in \mathbb{R} \) are the structure factors of \( g \). We let \( X := \sum_{k=1}^{L} h_k \), where \( L \leq K \) with no loss of generality and \( L < \infty \). Given a precision parameter \( \epsilon > 0 \), evolution time \( t \geq 0 \), and initial state \( | \psi \rangle \), the goal is to approximate \( U := e^{iX} \) by a unitary \( W \) such that

\[
\| (e^{iX} - W) | \psi \rangle \| \leq \epsilon .
\]

\( \| \cdot \| \) is the Euclidean norm of the state \( | \psi \rangle \). \( W \) admits the decomposition

\[
W = \prod_{n=1}^{N} e^{t_n h_{k_n}} ,
\]

where \( t_n \in \mathbb{R} \) and \( k_n \in [L] := \{ 1, 2, \ldots, L \} \).

In the following, the maximum is always taken over \( \lambda, \lambda' \in [0, t] \) and \( k \in [L] \) unless noted explicitly.

Main results.— Let \( r \geq 1 \) be an integer such that

\[
2(N_p)^2 \sum_{j=2p}^{\infty} (f_j N_p/r)^j t^{j+1} \beta_{j+1} \leq \epsilon ,
\]

where \( N_p := 2L5^{p-1}, p \geq 1 \) is an arbitrary integer, \( \beta_j := \max \| [\hat{h}_{k_1}, \ldots, \hat{h}_{k_j}] \ldots \| U(\lambda) \langle \psi | \rangle \| \), and \( f_j := 2 \) if \( j \leq N_p \) or \( f_j := 6N_p/j \) if \( j \geq N_p \). Then, there is a unitary \( W \) that approximates \( U \) as in Eqs. (2) and (3) and the number of terms in the product is \( N = r N_p \).

When the dimension of \( g \) is finite and if \( \epsilon t \geq \gamma \), then

\[
N = O \left( 5^{2p} L^{2\beta} \beta y \frac{t}{\gamma} \right) ,
\]

where

\[
\beta := \max_{k,k' \in g} \sum_{k''=1}^{K} |\gamma_{k,k'}^{k''}| ,
\]

and \( y := \max \| \hat{h}_k U(\lambda) \langle \psi | \rangle \| \).

Proofs.— Following Suzuki [3, 4], we define the unitary

\[
W_2(\lambda) = \prod_{k=1}^{L} e^{\lambda h_k/2} 1_{[0, t]} ,
\]

and the recursion relation (for integer \( p \geq 1 \))

\[
W_{2p+2}(\lambda) = (W_{2p}(s_p \lambda))^2 W_{2p}((1 - 4s_p \lambda)W_{2p}(s_p \lambda))^2 .
\]

The constants are \( s_p = 1/(4 - 1/(2p+1)) \). Similarly, we can write \( W_{2p}(\lambda) = V_{N_p} \ldots V_1 \), where each unitary \( V_n \) is of the form \( e^{(s'_n \lambda) h_{k_n}} k \) and \( k_n \in [L] \). The number of unitaries in the product results from the recursion and is \( N_p = 2L5^{p-1} \), and the coefficients \( s'_n \in \mathbb{R} \) satisfy \( |s'_n| < 1 \).

The operator \( \varepsilon_{2p}(\lambda) := W_{2p}^\dagger U(\lambda) = W_{2p}^\dagger \), where

\[
U(\lambda) := e^{iX} \quad \text{and} \quad \lambda \in [0, t],
\]

will provide information about the accuracy of the approximations \( W_{2p} \). Our first goal is then to find an upper bound of \( \varepsilon_{2p}(\lambda) := \| \varepsilon_{2p}(\lambda) | \psi \rangle \| \), where \( | \psi \rangle \) denotes some initial quantum state. Since \( \varepsilon_{2p}(\lambda) = \int_0^\lambda d\lambda' \partial_{\lambda'} \varepsilon_{2p}(\lambda') \), we obtain

\[
\varepsilon_{2p}(\lambda) = \int_0^\lambda d\lambda' W_{2p}^\dagger (\lambda') W_{2p}(\lambda' U(\lambda')) \|
\]

and then

\[
\varepsilon_{2p}(\lambda) \leq \lambda \max \| f_{2p}(\lambda') U(\lambda') | \psi \rangle \| .
\]

The operator \( f_{2p}(\lambda) \) can be obtained from the chain rule:

\[
f_{2p}(\lambda) = X - \sum_{n=1}^{N_p} s'_n V_{N_p} \ldots V_{n+1} \hat{h}_{k_n} V_{n+1}^\dagger \ldots V_{N_p}^\dagger .
\]
From the Lie algebra property, \( V_n \hat{h}_k V_n^\dagger = \mathbb{I} + \langle s'_n, \lambda \rangle [\hat{h}_k, V_n] + \langle s'_n, \lambda \rangle^2 [\hat{h}_k, [\hat{h}_k, V_n]]/2 + \ldots \). Then, Eq. 8 is a combination of nested commutators of those \( \hat{h}_k \) appearing in \( X \) so that

\[
f_{2p}(\lambda') = \sum_{k=1}^{\infty} c_k(\lambda') \hat{h}_k.
\]

The results in 3 imply that the lowest degree of the Taylor series of \( \varepsilon_{2p}(\lambda) \), for \( \lambda \to 0 \), is \( 2p + 1 \). It follows that the lowest degree in a Taylor series of the coefficients \( c_k(\lambda') \in \mathbb{R} \) is \( 2p + 1 \) and

\[
f_{2p}(\lambda') = \sum_{j=2p}^{\infty} \lambda^j \hat{r}_j.
\]

Each \( \hat{r}_j \in \mathfrak{g} \) results from sums of nested commutators of length \( j + 1 \), e.g., \([\hat{h}_{k_1}, [\hat{h}_{k_2}, \ldots, [\hat{h}_{k_j}, \ldots]]] \), with each \( k_i \in [L] \). The maximum number of possible nested commutators of such length involved in \( \hat{r}_j \) is bounded by

\[
N_p \left( N_p + j \right) + 1
\]

The factor \( N_p \) results from the sum of at most \( N_p \) transformations of the \( \hat{h}_k \) when using Eq. 8 and the binomial coefficient is the number of possible ways of partitioning \( j + 1 \) in \( N_p \) parts.

Since \( N_p \geq 5 \) for \( p \geq 2 \), and \( j \geq 2 \), Eq. 11 can be bounded by \( 2^{j+1}(N_p)^{j+2} \). When \( j + 1 \leq N_p \), we can then obtain \( \| \hat{r}_j U(\lambda') | \psi \rangle \| \leq 2^{j+1}(N_p)^{j+2} \beta_{j+1} \), where

\[
\beta_j = \max \| [\hat{h}_{k_1}, [\hat{h}_{k_2}, \ldots, [\hat{h}_{k_j}, \ldots]]] U(\lambda') | \psi \rangle \|
\]
is strongly dependent on the structure of the algebra. When \( j + 1 > N_p \), we can obtain an improved bound because nested commutators of length \( j + 1 \) must involve the same \( \hat{h}_k \) more than once. Let \( j + 1 = lN_p + l' \), with \( l \geq 1 \) and \( l' < N_p \) being nonnegative integers. Then, in determining each \( \hat{r}_j \) there is also a constant factor that is bounded by \((1/(l+1))^{l'}(1/l!)^{N_p-l'}\) due to the Taylor series of each transformation \( V_{N_p} \ldots V_{N_p + 1} \hat{h}_k V_{N_p + 1}^\dagger \ldots V_{N_p}^\dagger \) in Eq. 8. This constant corresponds to the case in which the nested commutator of length \( j + 1 \) results from the \((l + 1)\)th order in the Taylor series of \( \mathbb{L}' \) operators \( V_n \) and the \( l \)th order in the Taylor series of the remaining \( N_p-l' \) operators \( V_n \). This factor is easily bounded by \((1/(l!)^{N_p})\) and then \( \| \hat{r}_j U(\lambda') | \psi \rangle \| \leq \langle \mathbb{I}/l! \rangle^{N_p} 2^{j+1}(N_p)^{j+2} \beta_{j+1} \). We can use Stirling’s approximation and \( l \leq j/N_p \) to obtain \( 1/l! \leq (e/l)! l \leq (3N_p/j)^{j/N_p} \). These bounds together with Eqs. 11 and 11 now imply

\[
\varepsilon_{2p}(\lambda) \leq 2(N_p)^2 \sum_{j=2p}^{\infty} \lambda^j \beta_{j+1} (f_j N_p)^j \beta_{j+1} \tag{12}
\]

where \( f_j = 2 \) if \( 2p \leq j < N_p \) and \( f_j = 6N_p/j \) if \( j \geq N_p \). The case of \( \beta_j = 0 \) for all \( j \), corresponds to a commutative algebra and the error is exactly 0 in that case. The interesting case is when some \( \beta_j > 0 \) and from now on we assume that there exists \( \lambda > 0 \) such that Eq. 12 converges and is bounded.

To find an approximation of \( U = e^{iX} \), \( t \geq 0 \), we split \( t \) into \( r \) segments of size \( \lambda = t/r \). The subadditivity property of errors implies \( (\| U - W \| | \psi \rangle \| \leq r \varepsilon_{2p}(t/r) \). We define \( W := (W_{2p}(t/r))^r \). Then, \( r \varepsilon_{2p}(t/r) = 2(N_p)^2 \sum_{j=2p}^{\infty} (f_j N_p)^j t^{j+1} \beta_{j+1} \) and for precision \( \epsilon > 0 \), it suffices to satisfy \( r \varepsilon_{2p}(t/r) \leq \epsilon \) [Eq. 11]. The total number of exponentials in \( W \) is \( N = rN_p \); this proves our first result.

When the dimension of the Lie algebra is finite, it is useful to obtain \( \beta \) as in Eq. 11 and \( y = \max \| \hat{h}_k U(\lambda') | \psi \rangle \| \). It follows that \( \beta_{j+1} \leq \beta_j y \), and, since \( f_j \leq 6 \) for all \( j \), Eq. 12 implies

\[
\varepsilon_{2p}(\lambda) \leq (N_p y/\beta) \sum_{j=2p}^{\infty} (6N_p \beta)^j \beta_{j+1} \tag{13}
\]

To satisfy \( r \varepsilon_{2p}(\lambda) \leq \epsilon \), it suffices to choose

\[
r = \left[ 5^{p+2} L^{1+1/\beta} y^{1/\beta} t^{1+1/\beta} / \epsilon \right] \tag{14}
\]

This assumes that \( yt \geq \epsilon \) so that \( \lambda = t/r \) is sufficiently small for Eq. 12 to converge. Multiplying Eq. 13 by \( N_p \) gives \( N \) in Eq. 5 and proves our second result.

Below we obtain \( N \) for the approximation of the evolution operator of various quantum systems.

**Applications.**– Similar results to those in 3 can be essentially recovered if we assume that each \( \hat{h}_k \) in \( X \) is a bounded operator acting on a finite-dimensional Hilbert space 27. Those results consider the worst-case scenario and do not exploit certain structures of the commutation relations in the algebra. Thus, to emphasize the importance of our results, we first provide a Trotter-Suzuki approximation for certain finite-dimensional Lie algebras that is well suited to the case of continuous-variable quantum systems. In all our examples, \( X = -iH \), where \( H \) is the Hamiltonian of the system. Then \( U \) corresponds to the evolution operator and our goal is to find a product formula that approximates it.

We consider first the QHO, \( H = (p^2 + \hat{x}^2)/2 \), where \( \hat{p} \) and \( \hat{x} \) are the momentum and position operators, respectively (\( h = 1 \)). The operators \( i\hat{p}^2 \) and \( i\hat{x}^2 \), together with \( i\hat{x} \hat{p} \) := \( i\hat{x} \hat{p} + \hat{p} \hat{x} \), are a basis of the \( sp(2) \) Lie algebra of dimension \( K = 3 \); \( [i\hat{x}^2, i\hat{p}^2] = -2i(\hat{p} \hat{x} - \hat{x} \hat{p}) \), \( [i\hat{x}^2, i\hat{x} \hat{p}] = -4i\hat{x}^2 \), and \( [i\hat{p}^2, i\hat{x} \hat{p}] = 4i\hat{p}^2 \). These commutation relations easily follow from the canonical commutation relation \( [\hat{x}, \hat{p}] = i \), and then \( \beta = (1/2) \). The results in 3 cannot be directly applied to this case as \( \hat{p} \) and \( \hat{p} \) are unbounded operators. If \( |\psi\rangle = \sum_{m=0}^{\infty} c_m |\phi_m\rangle \), where \( |\phi_m\rangle \) are normalized eigenstates of \( H \) of eigenvalue
m + 1/2, then \( y \leq \max_{k,m} \| h_k \phi_m \| \) and \( y = O(m') \). This follows from the well-known properties of \( \hat{x} \) and \( \hat{p} \), where \( \hat{x} \phi_m = (\sqrt{m} \phi_{m-1}) + \sqrt{m+1} \phi_{m+1} / \sqrt{2} \) and \( \hat{p} \phi_m = -i (\sqrt{m} \phi_{m-1} - \sqrt{m+1} \phi_{m+1} / \sqrt{2} \). For precision \( \epsilon \), the number of terms in the approximation \( W \) of \( U \) results from Eq. (15) and simple calculations show

\[
N = O \left( 5^{2p} \left( m'/\epsilon \right)^{3p} t^{1+\frac{1}{2p}} \right),
\]

where we also used \( L = O(1) \). We can choose an optimal value of \( p \) that minimizes the value of \( N \) in Eq. (15). This occurs when \( p \approx \sqrt{\log(m't/\epsilon) / \log(5)} \) and then \( N = O(t \exp(\sqrt{\log(m't/\epsilon)})) \). Note that \( N \) is subpolynomial in \( m' \), i.e., \( N'/(m')^\alpha \) approaches 0 in the limit of large \( m' \) for any \( \alpha > 0 \). This result suggests that a subexponential quantum speedup can be attained in a quantum-computer simulation of \( U \) in the gate model. We showed that this is possible in [22].

We now consider the more general case of \( M \) coupled QHOs, where the Hamiltonian is, for example,

\[
H = \frac{1}{2} \sum_{i=1}^{M} (\hat{p}_i^2 + \hat{x}_i^2) - \sum_{i

It is well known that the operators appearing in \( X \) generate the \( sp(2M) \) Lie algebra of dimension \( K = M(2M+1) \). The structure of the factors of the algebra follow from the canonical commutation relations \( [\hat{x}_i, \hat{p}_j] = i \delta_{ij} \) and \( [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \), where \( \delta_{ij} \) is the Kronecker delta. As in the previous case, these factors imply \( \beta = O(1) \) [24]. With no loss of generality, the evolved state \( U(\lambda') | \psi \rangle \) is a linear combination of states \( | \phi_1, \ldots, \phi_{m_M} \rangle \). We will assume that there is \( m' \) such that, if we set \( m_i \leq m' \) for all \( i \) and \( \lambda \), then the approximation error induced by this assumption in the evolved state is negligible. Note that \( m' \) determines a local “energy scale”, as the expected value of \( (\hat{p}^2 + \hat{x}^2) / 2 \) in the evolved state is \( O(m') \). Then \( y = O(m'), L = O(M^2) \), and the number of terms in the approximation \( W \) of \( U \) given by Eq. (5) is

\[
N = O \left( 5^{2p} \left( m'/\epsilon \right)^{3p} (M^4 t)^{1+1/2p} \right).
\]

The optimal value of \( p \) that minimizes \( N \) can be obtained as before and gives \( N = O(M^4 t \exp(\sqrt{\log(M'M'/\epsilon)})) \), which is subpolynomial in \( m' \). We note that a similar analysis and result applies for those \( X \) (and corresponding Hamiltonians) that are more general linear combinations of the generators of \( sp(2M) \).

To demonstrate our result when the dimension of the Lie algebra is infinite, we apply our bound to the case where \( H = (\hat{p}^2 + \hat{x}^2) / 2 \), for integer \( q > 2 \). The Lie algebra generated by \( i\hat{p}^2 \) and \( i\hat{x}^2 \) is infinite dimensional. To bound the errors in the approximation of \( U \), it is necessary to study the properties of nested commutators for this case. We note that \( [x^k, x_j^l p^m] \) are polynomials of \( x \) and \( \hat{p} \). We will use induction to show that the degree of this polynomial is \( k + l + m - 2 \) and, in particular, the degree associated with \( x \) is \( k + l - 1 \) and the degree associated with \( \hat{p} \) is \( m - 1 \). When \( k = m = 1 \), we have \( [\hat{x}, \hat{x}^l \hat{p}^m] = \hat{x}^l [\hat{x}, \hat{p}] = i \hat{x}^l \), so the statement is valid in this case. Also, it is simple to show \( [\hat{x}^k, \hat{x}^l \hat{p}^m] = [\hat{x}^k, \hat{x}^l \hat{p}^m \hat{p}] + ik\hat{x}^{l+k} \hat{p}^m \hat{x}^{k-1} \) and \( [\hat{x}^{k+1}, \hat{x}^l \hat{p}^m] = \hat{x}^{k+1} \hat{x}^l \hat{p}^m + ik\hat{x}^{k+l} \hat{p}^m \hat{x}^k \), so that increasing \( k \) or \( m \) by 1 only increases the degree of \( \hat{x} \) or \( \hat{p} \) by 1, respectively. This demonstrates the induction step. These properties also imply that if we commute a polynomial in \( \hat{x} \) and \( \hat{p} \) with \( \hat{p} \), then the degree of \( \hat{x} \) is reduced by 1 while the degree of \( \hat{p} \) is increased by 1. Also, if we commute such a polynomial with \( \hat{x}^q \), the degree of \( \hat{x} \) is increased by \( q - 1 \) while the degree of \( \hat{p} \) is reduced by 1. This is a useful observation because the operators \( \hat{r}_j \) in Eq. (10) result from nested commutators of \( i\hat{x}^q \) and \( i\hat{p}^2 \) in this case. In particular, the only nonzero nested commutators of length \( j + 1 \) are those for which the number of appearances of \( \hat{x}^q \) is less than or equal to \( (j + 2)/2 \); otherwise the degree of \( \hat{p} \) would be negative leading to an inconsistency. Then, the largest degree of the polynomial generated by a nested commutator of length \( j + 1 \) is upper bounded by \( d_j = (q - 2)(j + 2)/2 + 2 \), which was obtained for the worst case scenario in which the number of appearances of \( \hat{x}^q \) is at most, \( (j + 2)/2 \).

Without any loss of generality, \( U(\lambda') | \psi \rangle = \sum_\lambda c_\lambda | \phi_\lambda \rangle \) and we assume that there exists \( m' \) such that, if we cut off the sum at \( m \leq m' \), the error induced by this approximation is negligible or \( O(\epsilon) \) for all \( \lambda \in [0, t] \). We will then bound the approximation error by assuming that \( U(\lambda') | \psi \rangle \) has no support in those states \( | \phi_\lambda \rangle \) for \( m > m' \). This poses no problem as the additional error factor in \( \epsilon_{2p} \) is still \( O(\epsilon) \). The value of \( m' \) determines the relevant energy scale of the problem—see below. Then,

\[
\beta_{j+1} \leq \frac{2^j \max_{0 \leq d_j, 0 \leq m \leq 2m'} \| T_j | \phi_m \|}{2^{j/2} (m' + d_j)^{d_j/2}},
\]

where \( T_j \) is a product of \( l \) operators \( \hat{x} \) and \( d_j - l \) operators \( \hat{p} \), in some order. To bound the error in the approximation of \( U \) by \( W \) we first use Eq. (10) in Eq. (12). This error depends on \( q \) and, for large \( q \), it can diverge. Nevertheless, if we assume \( 2 \leq q \leq 6 \), a few algebraic manipulations using Eq. (12) imply

\[
\epsilon_{2p} (\lambda) \leq \sum_{j=2p}^\infty (c AN_p^2)^{j+1} (m')^{j+1/2p} + \frac{2}{2p},
\]

where \( c > 1 \) is a constant. We can obtain \( r \) by setting \( r = 2 \) and then use it to obtain \( N \). Then, the number of exponentials in \( W \) in this case is

\[
N = O \left( 5^{3p} \left( m'/\epsilon \right)^{3p} (M^4 t)^{1+1/2p} \right).
\]

We note that Eq. (17) is a much better bound for \( N \) than that obtained if we replace the exponent of \( m' \) by
\((q/2)(1 + 1/2p)\) in the same equation. Such an exponent would be obtained if we assumed that the norm of the effective operator \(\hat{x}'\) could be replaced by \(O(m'^2)\) and then use the results in \(\mathbb{R}\). Our result for \(N\) also suggests a polynomial quantum speedup with respect to classical methods for simulating the evolution operator, as the dependence of \(N\) with \(m'\) is sublinear when \(q \leq 5\) and subquadratic when \(q = 6\).

We note that both, the classical and quantum algorithm complexities, depend on the same value of \(m'\) that determines the dimension of the relevant Hilbert subspace associated with the evolved state. It may then be useful to understand the dependence of \(m'\) in the special case where \(|\psi\rangle = |\phi_m\rangle\). For example, it is simple to show \((\hat{x}'^2 + \hat{p}'^2)/2 \leq I + (\hat{p}'^2 + \hat{x}'^2)/2\) when \(q\) is even. Then, \langle m | U^{1}(\lambda) (\hat{x}'^2 + \hat{p}'^2) U(\lambda) | m \rangle = O(m'^2)\) and we can use Markov’s inequality to show that the support of \(U(\lambda) | \phi_m \rangle\) in the space spanned by \(| \phi_m \rangle\), for \(m' = O(m'^2)\), is bounded by an arbitrarily small constant. (We can improve this bound by using inequalities that involve moments of higher order.) We can use this value of \(m'\) in Eq. (17) for this particular case.

Conclusions.– We presented an improved product formula to approximate the evolution operator of various quantum systems that exploits the structure of commutation relations of the associated Lie algebra. We applied this formula to examples of bosonic quantum systems and the results suggest that quantum-computer simulations of such systems can be done significantly more efficiently than classically possible.

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[25] The number of exponentials given by our Eq. (3) can actually be smaller than that obtained in \(\mathbb{R}\). For example, when \(\|\hat{h}_0\| \leq 1\) and \(\epsilon\) and \(t\) are constant, we obtain \(N = O(5^{2p}L^{2+1/p})\) while \(\mathbb{R}\) implies \(N = O(5^{2p}L^{3+1/2p})\).