Higher-Order Methods for Quantum Simulations

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To efficiently implement many-particle quantum simulations on quantum computers we develop and present methods for inverting the Campbell-Baker-Hausdorff lemma to 3rd and 4th order in the commutator. That is, we reexpress \( \exp \left( -i \sum H_i \Delta t \right) \) as a product of factors \( \exp (-i H_1 \Delta t), \exp (-i H_2 \Delta t), \ldots \) which is accurate to 3rd or 4th order in \( \Delta t \).

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Quantum computers have generated much interest recently, largely due to the result by Shor \[1\] that they can factor integers in an amount of time that grows polynomially with the size of the integer. This can be compared to factorization on a classical computer, where the time it takes to factor a number grows exponentially with the input size. In addition to Shor’s factorization algorithm, simulations of quantum systems have also been shown to be possible in polynomial time \[2\]. Indeed, this was the first area for which it was proposed that quantum computers could fundamentally be more powerful (i.e. much faster) than classical computers \[2\].

From a theoretical standpoint, a quantum computer is a quantum system with a \( 2^n \)-dimensional Hilbert space. Pairs of states in the system are defined to be ‘qubits’. The canonical example of such a system is a set of \( n \) spins. Each spin consists of two states, so each spin can represent a qubit and the Hilbert space of the system is \( 2^n \)-dimensional. The equivalent of a logical gate on a classical computer is an operator acting on a set of qubits on a quantum computer.

This letter focuses on a problem which concerns simulational issues in quantum computation. A simulation of a quantum mechanical system on a quantum computer consists of applying an operator \( \exp (-iHt) \) on a set of qubits, where \( H \), the Hamiltonian of the system of interest, is suitably encoded (and discretized) to act on the set of qubits. For many-particle systems \( H \) is a sum of terms. For instance, the Hubbard model Hamiltonian, used in the study of high-\( T_c \) superconductivity, can be written \[3\] as the sum

\[
H = \sum_{\sigma} \sum_{i} V_{0} n_i \sigma + \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma}
\]

(1)

where \( V_{0} \) is the strength of the potential, and \( n_i \sigma \) is the operator for the number of fermions of spin \( \sigma \) at site \( i \). In the second (kinetic energy) term, the sum \( \langle i,j \rangle \) indicates all neighboring pairs of sites, \( t_{ij} \) is the strength of the “hopping”, and \( c_{i \sigma}, c_{i \sigma}^\dagger \) are annihilation and creation operators, respectively, of a fermion at site \( i \) and spin \( \sigma \). This model gives an example in which a full simulation on a classical computer is impossible due to the exponential increase in the size of the Hilbert space of the quantum system with the number of lattice sites.

The canonical quantum computer cannot act on all spins at once \[4\]. Therefore, it becomes necessary to find ways of approximating the evolution operator, which is the exponential of a sum of operators (with a Hamiltonian such as that in Eq. (1)) as a product of operators each acting on a subspace of the Hilbert space. To second order, for instance, we could use the approximation

\[
\left( e^{-iH_1 \Delta t} e^{-iH_2 \Delta t} \ldots e^{-iH_N \Delta t} \right) \approx e^{-i \sum (H_1 + H_2 + \ldots + H_N) \Delta t + O[(\Delta t)^3]}
\]

(2)

where the \( e^{-iH_i \Delta t} \) act on a subspace of the Hilbert space.

To find higher order approximation methods, we want to reexpress \( \exp \left( \sum_{n=1}^{N} A_n \right) \) as a product of individual \( \exp (A_n) \)'s. In order to do this, we must invert the Campbell-Baker-Hausdorff formula. To 5th order, the Campbell-Baker-Hausdorff formula is

\[
\exp (aA_1) \exp (aA_2) = \exp \left[ a (A_1 + A_2) + \frac{1}{2} a^2 A_{12} + \frac{1}{6} a^3 (A_{1112} + A_{221}) \right.
\]

\[
+ \frac{1}{24} a^4 A_{1221} - \frac{1}{720} a^5 (A_{11111} - 2A_{21112} - 6A_{11221} - 6A_{22112} - 2A_{12221} + A_{22221}) + O (a^6) \right] \]

(3)

where

\[
A_{k_1 \ldots k_m} \equiv [A_{k_1}, [A_{k_2}, \ldots [A_{k_m}, A_{n}] \ldots]]
\]

(4)

As a strategy for finding approximation methods, we pick a fundamental ordering of the product of exponentials with parameters allowing for transposes of the entire product as well as raising all the exponentials in the fundamental unit to the same power. By iterating the Campbell-Baker-Hausdorff formula, we can get an expression for this fundamental unit in terms of a single exponential

\[
\left( e^{aA_1} e^{aA_2} \ldots e^{aA_N} \right)^\alpha = \exp \sum_{p=1}^{\infty} \alpha a^p B_N^p
\]

(5)

which defines the \( B_N^p \) in terms of the \( A_n \). Here, \( p \) is an exponent on \( a \), and a label on the matrices \( B_N^p \).
Now combine a succession \( i = 1, \ldots, I \) of fundamental units with parameters \( a_i \) and \( \alpha_i \). Again iterating Campbell-Baker-Hausdorff gives

\[
\exp \left( \sum_{p=1}^{\infty} \alpha_1 a_1^p B_N^p \right) \ldots \exp \left( \sum_{p=1}^{\infty} \alpha_I a_I^p B_N^p \right) = \exp \left( \sum_X \sigma_X^X B_N^X \right)
\]  

(6)

The \( B_N^X \) are generated from the \( B_N^p \) by commutation. \( X \) represents a label \( pq \ldots rs \) where

\[
B_N^{pq \ldots rs} = [B_N^p, [B_N^q, \ldots [B_N^r, B_N^s] \ldots ]]
\]  

(7)

\( B_N^{pq \ldots rs} \) is of order \( p + q + \ldots + r + s \). Up to 5th order we can take

\[
X \in \{1; 2, 3, 12, 4, 13, 112, 5, 14, 23, 113, 221, 1112\}
\]  

(8)

These \( B_N^X \) span the space of the \( B_N^p \)’s and their commutators to 5th order and for \( N \geq 2 \) they are independent. The \( \sigma_X^p \) are defined in terms of \( \alpha_1 \) and \( a_i \) by Eq. (8). Here again, the \( X \)’s are labels. After some calculation, the Campbell-Baker-Hausdorff formula, Eq. (8), gives the equations

\[
\sigma_I^p = \sum_{i=1}^{I} \alpha_i a_i^p
\]  

(9)

for \( p = 1, \ldots, 5 \),

\[
\sigma_I^{pq} = -\frac{1}{2} \sigma_I^p \sigma_I^q + \frac{1}{2} \sum_{i=1}^{I} a_i^{q-p} \left[ (\sigma_I^p)^2 - (\sigma_I^{p-1})^2 \right]
\]  

(10)

for \( pq = 12, 13, 14, 23 \),

\[
\sigma_I^{ppq} = -\frac{1}{2} \sigma_I^p \sigma_I^{pq} - \frac{1}{6} (\sigma_I^p)^2 \sigma_I^q
\] 

\[ + \frac{1}{6} \sum_{i=1}^{I} a_i^{q-p} \left[ (\sigma_I^p)^3 - (\sigma_I^{p-1})^3 \right]
\]  

(11)

for \( ppq = 112, 113, 221 \), where \( \sigma_I^{112} \equiv -\sigma_I^{12} \)

\[
\sigma_I^{1112} = -\frac{1}{2} \sigma_I^{11} \sigma_I^{112} - \frac{1}{3} (\sigma_I^{11})^2 \sigma_I^{12} - \frac{1}{24} (\sigma_I^{11})^3 \sigma_I^{12}
\] 

\[ + \frac{1}{24} \sum_{i=1}^{I} a_i \left[ (\sigma_I^{11})^4 - (\sigma_I^{11-1})^4 \right]
\]  

(12)

For approximations to \( \exp \left( \sum_{n=1}^{N} A_n \right) \), we require all \( \sigma_I^X = 0 \) except for \( \sigma_I^1 \) which is the coefficient of \( B_N^1 = \sum_{n=1}^{N} A_n \), and which should be greater than zero.

An interesting feature of 3rd order methods is that they require at least one inverse, i.e. they require backward time evolution during part of the method. This follows immediately from Eq. (1) with \( p = 3 \). It can also be proved using Eq. (1) with \( p = 3 \) and \( p = 4 \) that 4th order methods must have at least two inverses.

Our basic method to solve Eqs. (11-13) is to pick values of \( \alpha_1 \) and \( a_i \) and see if they satisfy the equations. To do this we must restrict the number of fundamental units by fixing \( I \). We also take the \( \alpha_i \)’s to be \( \pm 1 \) and restrict the range of the \( a_i \)’s.

We start with Eq. (1), since, in this equation, order with respect to \( i \) does not matter. So, for a given set of values, we need to consider only one permutation, not all permutations of the values. This greatly reduces the size of the search.

Furthermore, we start by considering \( p = 1 \) and 3, since it is only the sign of \( \alpha_1 a_1 \) that matters in these equations. This means we can consider only the sign of the combination \( \alpha_1 a_1 \), and not the signs of \( \alpha_i \) and \( a_i \) individually. This reduces the search further. These equations are particularly restrictive for the case of few inverses.

After solving the \( p = 1 \) and 3 equations, we introduce separate signs for the \( \alpha_i \)’s and \( a_i \)’s and solve the equation with \( p = 2 \), and \( p = 4 \) for the 4th order case.

Finally, into the restricted set of solutions to Eq. (1) we introduce permutations of the \( \alpha_i \)’s and \( a_i \)’s with respect to the index \( i \) and solve Eqs. (11-13).

We find a larger number of solutions than we can easily present. We want to present solutions which are in some sense optimal. To do this, we consider the form of the operator resulting from a given method

\[
\prod_{j=1}^{I} \left( e^{-ia_j A_1 \Delta t} e^{-ia_j A_2 \Delta t} \ldots e^{-ia_j A_N \Delta t} \right)^{\alpha_j}
\]  

(13)

where \( \Delta t \ll 1 \) is a time step, \( o \) is the order of the method, and

\[
r = \sum_{X} \sigma_X^X B_N^X
\]  

(14)

where \( X \in \{4, 13, 112\} \) for a 3rd order method and \( X \in \{5, 14, 23, 113, 221, 1112\} \) for a 4th order method.

\( r \) is an error which takes values in the vector space of the commutators for which we do not have a metric. Therefore, we make an ad hoc choice of basis to be discussed elsewhere. This allows us to replace \( r \) by a single real scalar \( R \). The error from the method can then be taken to be

*After this work was completed, we became aware that this point had also been noted in [8].
where \( n \) is the number of times we apply the approximate method.

If the physical time we want to simulate is \( T_p \), then
\[
T_p = n D \Delta t
\]
where \( D \equiv \sigma^\dagger \) is given by the method.

The computer time it takes for a given simulation can be written
\[
T_c = n I N t_g + n L N t_s
\]
where \( I \) is the number of fundamental units in the method and \( N \) is the number of terms in a unit, \( t_g \) is the time it takes to make a gate change,
\[
L \equiv \sum_{i=1}^{J} |a_i|
\]
so that \( L N \) is the total time the gates are applied for in the method. The time an individual gate is applied for will be \( t_g = b \Delta t \), where \( b \) is a proportionality constant dictated by the actual couplings in the quantum computer hardware.

Using Eqs. (15) and (16), the computer time can be rewritten
\[
T_c = \left( \frac{T_p^{n+1}}{E} \right)^{\frac{1}{2}} \left( \frac{G}{D} \right) \left( \frac{R}{D} \right)^{\frac{1}{2}} t_g + \frac{L b T_p}{D}
\]
where \( E \) is the number of terms we apply the approximate method.

To illustrate our methods, we have applied first, second, third and fourth order methods to the exactly solvable operator
\[
e^{-i \Delta t (\sigma_x + \sigma_y + \sigma_z)} = \left( C - \frac{1}{\sqrt{3}} S \frac{1}{\sqrt{3}} S \right) C + \frac{1}{\sqrt{3}} S
\]
where \( C \equiv \cos (\sqrt{3} \Delta t) \) and \( S \equiv \sin (\sqrt{3} \Delta t) \).

As a measure of the error, we took the differences \( \Delta \sigma_x, \Delta \sigma_y \) and \( \Delta \sigma_z \) between the \( \sigma_x, \sigma_y \) and \( \sigma_z \) components of the exact solution and those of the results of our methods. We then calculated the error
\[
E = \sqrt{(\Delta \sigma_x)^2 + (\Delta \sigma_y)^2 + (\Delta \sigma_z)^2}
\]

In Fig. (1), we plot the logarithm of the error as a function of the logarithm of the time that the system was evolved for. The first order method results are uppermost and higher order results lie underneath each other with fourth order results being the lowermost plotted. \( \Delta t = 0.01 \) for all methods.

![FIG. 1. A measurement of the accuracy of our results. Plotted is the log(error) of (from top to bottom) first, second, third and fourth order approximation methods as a function of log(time). Note that for the fourth order method, the error never grows larger than \( 10^{-3} \).](image-url)
Notice that the first order error oscillates once it reaches order 1. The rest of the errors remain small throughout the simulation, with the fourth order error remaining below $10^{-3}$ for the entire evolution.

The error for all methods goes as $nR(\Delta t)^{n+1}$, where $n$ is the number of times the method has been applied. Therefore, $\log E = \log n + \log \left[R(\Delta t)^{n+1}\right]$. For $\Delta t = 0.01$, this makes the $y$-intercept decrease roughly by order $-2$ as the order of the method increases. Since the time evolved is proportional to $n$, the slope of the errors is 1 for all methods.

As an example of how useful our approximations can be, let us consider a case in which we want to apply an approximation method for time $T = 1$ with total error $E = 10^{-4}$. For a first order method, this means that we require about 5000 applications of the method. For second order, we require about 30 applications. For our third order method, we need 2 applications. And for our fourth order method, we need less than 1 application of the method. This results in a reduction of orders of magnitude in the computational cost of a given simulation.

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