Hamiltonian Dynamics using Linear Combination of Unitaries

Harsh Rathod

21st May, 2026

Tutor: Sahil Ugale

Professors: Dr. Felix Motzoi and Dr. Markus Heinrich

Berry et.al - Simulating hamiltonian dynamics with a truncated Taylor series. Physical Review Letters, 114(9), March 2015.

LA-UR-14-22745, MIT-CTP #4618

Simulating Hamiltonian dynamics with a truncated Taylor series

Dominic W. Berry[1], Andrew M. Childs[2,3,4,5], Richard Cleve[2,5,6], Robin Kothari[2,6,7], and Rolando D. Somma[8]

[1]*Department of Physics and Astronomy, Macquarie University, Sydney, NSW 2109, Australia*
[2]*Institute for Quantum Computing, University of Waterloo, ON N2L 3G1, Canada*
[3]*Department of Combinatorics & Optimization, University of Waterloo, ON N2L 3G1, Canada*
[4]*Department of Computer Science, Institute for Advanced Computer Studies, and Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD 20910, USA*
[5]*Canadian Institute for Advanced Research, Toronto, Ontario M5G 1Z8, Canada*
[6]*School of Computer Science, University of Waterloo, ON N2L 3G1, Canada*
[7]*Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[8]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

(Dated: December 16, 2014)

We describe a simple, efficient method for simulating Hamiltonian dynamics on a quantum computer by approximating the truncated Taylor series of the evolution operator. Our method can simulate the time evolution of a wide variety of physical systems. As in another recent algorithm, the cost of our method depends only logarithmically on the inverse of the desired precision, which is optimal. However, we simplify the algorithm and its analysis by using a method for implementing linear combinations of unitary operations to directly apply the truncated Taylor series.

One of the main motivations for quantum computers is their ability to efficiently simulate the dynamics of quantum systems [1]. Since the mid-1990s, many algorithms have been developed to simulate Hamiltonian dynamics on a quantum computer [2–12], with applications to problems such as simulating spin models [13] and quantum chemistry [14–17]. While it is now well known that quantum computers can efficiently simulate Hamiltonian dynamics, ongoing work has improved the performance and expanded the scope of such simulations.

Recently, we introduced a new approach to Hamiltonian simulation with exponentially improved performance as a function of the desired precision [18]. Specifically, we presented a method to simulate a d-sparse, n-qubit Hamiltonian H acting for time $t > 0$, within precision $\epsilon > 0$, using $O(\tau \log(\tau/\epsilon)/\log\log(\tau/\epsilon))$ queries to H and $O(n\tau \log^2(\tau/\epsilon)/\log\log(\tau/\epsilon))$ additional two-qubit gates, where $\tau := d^2\|H\|_{\max}t$. This dependence on ϵ is exponentially better than all previous approaches to Hamiltonian simulation, and the number of queries to H is optimal [18]. (For simplicity, we refer to combinations of logarithms like those in the above expressions as logarithmic.) Roughly speaking, doubling the number of digits of accuracy only doubles the complexity.

The simulation algorithm of [18] is indirect, appealing to an unconventional model of query complexity. In this paper, we describe and analyze a simplified approach to Hamiltonian simulation with the same cost as the method of [18]. The new approach is easier to understand, and the reason for the logarithmic cost dependence on ϵ is immediate. The new approach decomposes the Hamiltonian into a linear combination of unitary operations. Unlike the algorithm of [18], these terms need not be

The main idea of the new approach is to implement the truncated Taylor series of the evolution operator. Similarly to previous approaches for implementing linear combinations of unitary operators [12, 13], the various terms of the Taylor series can be implemented by introducing an ancillary superposition and performing controlled operations. The time evolution is broken up into *segments*, each of which is short enough that the evolution can be accurately approximated using a number of terms in the Taylor series that is logarithmic in $1/\epsilon$. Each segment is then performed using *oblivious amplitude amplification* [18]. To make this work in the present context, we show that a more powerful *robust* version of amplitude amplification holds, where the target operation need not be unitary (and our proof of this is simpler than the proof for a weaker version in [18]). The complexity of the method is essentially given by the order at which the series is truncated times the number of segments.

Our algorithm can be applied to simulate various models of realistic systems, including systems of spins or fermions. It can also be used to implement other quantum algorithms [3, 19, 20]. We focus on the case of time-independent Hamiltonians for simplicity, but we also outline a straightforward application of our results to time-dependent Hamiltonians.

Specifically, we present a quantum algorithm that simulates the time evolution of a finite-dimensional Hamiltonian of the form

$$H = \sum_{\ell=1}^{L} \alpha_\ell H_\ell.$$

Primary aim using a Quantum Computer

- Simulate dynamics of a Quantum system
- More efficiently than a Classical computer !
- Trotterization

$$H = A + B \qquad U = e^{i(A+B)t} \qquad U = (e^{-i(A+B)t/r})^r$$

In general, $[A, B] \neq 0$

$$U_r = e^{-iAt/r} e^{-iBt/r} + O((t/r)^2)$$

After r steps,

$$\text{Error}(\epsilon) \approx r.(t/r)^2 = t^2/r$$
$$r \approx t^2/\epsilon = O(1/\epsilon)$$

- Even for higher order Trotter-Suzuki approximations, error scales polynomially
- Can we do better?

Linear Combination of Unitaries

- Decompose the Hamiltonian into a linear combination of Unitaries (H_l)
- Split the Evolution operator into r segments
- Approximate each segment with a Taylor expansion up to K[th] order
- Implement $\widetilde{U}$ (U_r)

Note:

The operator $\widetilde{U}$ may not necessarily be Unitary

$$H = \sum_{l=1}^{L} \alpha_l H_l \qquad U = e^{-iHt} = e^{\left(-iH\frac{t}{r}\right)^r}$$

$$U_r = e^{-iH\frac{t}{r}} \approx \sum_{k=0}^{K} \frac{1}{k!}\left(-iH\frac{t}{r}\right)^k = \sum_{k=0}^{K} \frac{1}{k!}\left(-\frac{it}{r}\left(\sum_{l=1}^{L}\alpha_l H_l\right)\right)^k$$

$$U_r \approx \sum_{k=0}^{K} \sum_{l_1,\ldots,l_k=1}^{L} \frac{(-it/r)^k}{k!} \alpha_{l_1}\ldots\alpha_{l_k} H_{l_1}\ldots H_{l_k} \qquad (1)$$

Extensively studied problem [1]: (where, $\beta_j > 0$ and each V_j is a Unitary)

$$\tilde{U} = \sum_{j=0}^{m-1} \beta_j V_j$$

Comparing with Eq. 1

$$\beta_j = \frac{(t/r)^k}{k!}\alpha_{l_1}\ldots\alpha_{l_k} \qquad V_j = (-i)^k H_{l_1}\ldots H_{l_k}$$

[1] R. Kothari, Ph.D. thesis, University of Waterloo (2014).

- Prepare the auxiliary qubit in a superposition state
- We can repeat this procedure multiple times for each segment U_r and thereby apply the Evolution operator

Note:
Probability of success is very low

Consider a m-dimensional unitary B to prepare the auxiliary state

$$B|0\rangle = \frac{1}{\sqrt{s}} \sum_{j=0}^{m-1} \sqrt{\beta_j} |j\rangle \qquad s \coloneqq \sum_{j=0}^{m-1} \beta_j$$

Implementing V_j as, for any $j \in \{0, 1, ..., m-1\}$

$$select(V)|j\rangle|\psi\rangle = |j\rangle V_j|\psi\rangle$$

Define:

$$W = (B^\dagger \otimes \mathbb{1})(select(V))(B \otimes \mathbb{1})$$

$$W|0\rangle|\psi\rangle = \frac{1}{s}|0\rangle\tilde{U}|\psi\rangle + \sqrt{1 - \frac{1}{s^2}}|\phi\rangle$$

where, $|\phi\rangle$ is a state whose auxilary state is orthogonal to $|0\rangle$

Finally, using $P \coloneqq |0\rangle\langle 0| \otimes \mathbb{1}$,

$$PW|0\rangle|\psi\rangle = \frac{1}{s}|0\rangle\tilde{U}|\psi\rangle$$

Probability of success is $1/s^2$

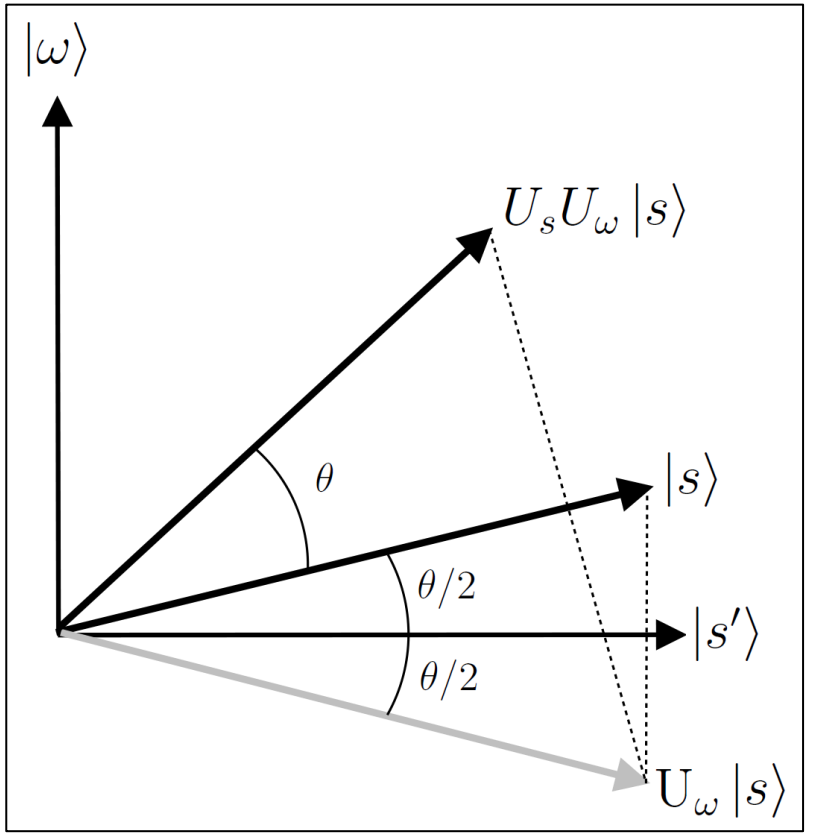
Recap: Grover's search algorithm (Amplitude Amplification)

- Initial state can split into the desired state and an orthogonal subspace with the remaining components
- Step 1: Reflect about the bad subspace
- Step 2: Reflect about the initial state
- Therefore, we end up rotating the initial state by θ where, $\theta/2$ is the initial angle

$$|\psi_i\rangle = sin\left(\frac{\theta}{2}\right)|Good\rangle + cos\left(\frac{\theta}{2}\right)|Bad\rangle$$

After p repetitions of Grover operator,

$$|\psi_f\rangle = sin\left(\frac{(2p+1)\theta}{2}\right)|Good\rangle + cos\left(\frac{(2p+1)\theta}{2}\right)|Bad\rangle$$



Oblivious Amplitude Amplification

- We can tune s by choosing the number of segments r
- This process is **oblivious** to the system state ψ
- Applying operator A is equivalent to implementing $U_r \approx \tilde{U}$ on the initial state ψ

Initial state to be amplified

$$W|0\rangle|\psi\rangle = \frac{1}{s}|0\rangle\tilde{U}|\psi\rangle + \sqrt{1-\frac{1}{s^2}}|\phi\rangle$$

For $s = 2$,

$$W|0\rangle|\psi\rangle = sin\left(\frac{\pi}{6}\right)|0\rangle\tilde{U}|\psi\rangle + cos\left(\frac{\pi}{6}\right)|\phi\rangle$$

Therefore, after one iteration of Amplitude Amplification results in

$$A|0\rangle|\psi\rangle = |0\rangle\tilde{U}|\psi\rangle$$

where, $A = -WRW^{\dagger}RW$

$A =$ (Reflect about intial state) (Reflect about bad subspace) (State prep)

$= -(\mathbb{1} - 2(W|0\rangle|\psi\rangle)(\langle\psi|\langle 0|W^{\dagger}))$ $(\mathbb{1} - 2|0\rangle\langle 0|)$ (W)

$= -W(\mathbb{1} - 2|0\rangle\langle 0|)W^{\dagger}$ $(\mathbb{1} - 2|0\rangle\langle 0|)$ (W)

$= -WRW^{\dagger}RW$

Only valid when $\tilde{U}$ is Unitary

Effect of Non-Unitarity

- Unitary operators are not closed under addition
- But if we are able to bound the error in $\widetilde{U}$ up to $O(\delta)$ then we can implement the evolution operator with an error of $O(\varepsilon)$ (where, $\varepsilon = r\delta$)

For $s \neq 2$ and $\tilde{U}$ being non-Unitary,

$$PA\,|0\rangle\,|\psi\rangle = |0\rangle \left(\frac{3}{s}\tilde{U} - \frac{4}{s^3}\tilde{U}\tilde{U}^{\dagger}\tilde{U}\right)|\psi\rangle$$

If $|s-2| = O(\delta)$ and $||\tilde{U} - U_r|| = O(\delta)$ then $||\tilde{U}\tilde{U}^{\dagger} - \mathbb{1}|| = O(\delta)$ and

$$||PA\,|0\rangle\,|\psi\rangle - |0\rangle\,U_r\,|\psi\rangle\,|| = O(\delta)$$

Topics not discussed here:

Time-dependent Hamiltonians
Gate complexity of implementing the above discussed operators

Summary

- Primary aim using a Quantum Computer
  - Simulate Quantum systems
  - Trotter-Suzuki algorithm
  - Error scales polynomially
- LCU
  - Express time-dependent Hamiltonian in terms of Unitaries
  - Break the Evolution operator into segments and approximate using Taylor expansion
  - Implement each segment $\widetilde{U}$
  - Oblivious Amplitude Amplification
- Effect of Non-Unitarity
- Time-dependent Hamiltonians
- Gate complexity

Benefits of LCU

- No special Hamiltonian form required
- Exponentially improved performance

For a d-sparse n-qubit Hamiltonian H acting for time t,

Number of queries to the Hamiltonian is of the order

$$N_{\mathrm{H}} \approx O\left(\frac{\tau \log(\tau/\epsilon)}{\log(\log(\tau/\epsilon))}\right)$$

and an additional two-qubit gates of the order

$$N_{\mathrm{aux}} \approx O\left(\frac{n\tau \log^2(\tau/\epsilon)}{\log(\log(\tau/\epsilon))}\right)$$

where, $\tau := d^2||\mathrm{H}||_{\max} t$

Doubling the number of digits of accuracy only doubles the complexity !

- Not limited to Hamiltonian Dynamics, also used in Quantum Machine Learning, Thermal state preparation, Quantum Differential Equation solvers, etc.

Can we do even better?

Qubitzation