Hamiltonian simulation with complexity polylogarithmic in the error

Dominic W. Berry* Rolando D. Somma† Richard Cleve‡

Abstract

Quantum algorithms for the simulation of quantum systems described by a Hamiltonian provide an exponential improvement in speed over classical algorithms when one considers scaling of the complexity in terms of the dimension. However, one key drawback is that the scaling in terms of the allowable error, ε, is relatively poor. Here we provide a new quantum algorithm whose scaling with respect to the allowable error is exponentially smaller than previous algorithms. That is, the complexity is polylogarithmic in $1/\varepsilon$, rather than polynomial. The algorithm's scaling with respect to other parameters—such as dimension and evolution time—also compares well with previous algorithms.

1 Introduction and problem definition

The simulation of physical systems provides a natural application where quantum computers can provide an exponential improvement over classical computers, and indeed this is the original reason why Feynman proposed the concept of a quantum computer [1]. Lloyd [2] showed how to efficiently simulate Hamiltonians that are expressible as a sum of simple interaction Hamiltonians.

We consider the problem of simulating d-sparse Hamiltonians acting on n qubits whose non-zero entries can be systematically determined. This was defined formally as a computational problem by Aharonov and Ta-Shma [3] in terms of an oracle that specifies the positions and values of the non-zero entries of the Hamiltonian H (this oracle is defined formally in Section 4). The input to the simulation problem includes an initial quantum state $|\psi\rangle$, evolution time t, and precision parameter ε, in addition to the oracle for H. The output should be a quantum state that corresponds (within trace distance ε) to unitary evolution of $|\psi\rangle$ under H for time t. In the case of time-independent Hamiltonians, the target final state is $e^{-iHt}|\psi\rangle$. In the case of time-dependent Hamiltonians, the final state is a solution to the Schrödinger equation.

2 Previous results

The problem that we consider was first proposed and investigated by Aharonov and Ta-Shma [3], who showed how to simulate sparse Hamiltonians by decomposing into a sum of 1-sparse Hamiltonians, yielding scaling that is polynomial in n (number of qubits), t (evolution time), and d

*Department of Physics and Astronomy, Macquarie University, Sydney, NSW 2109, Australia.
†Theory Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.
‡David R. Cheriton School of Computer Science and Institute for Quantum Computing, University of Waterloo.

(sparsity). A later development was improved decomposition methods [4, 5, 6] and application of high-order Trotter-Suzuki formulas to simulate the sum. This approach results in scaling that is close to linear with respect to the evolution time t, namely, $t^{1+O(1/\sqrt{\log t})}$. Note that this is $t^{1+o(1)}$, but not $t \operatorname{polylog} t$. An alternative approach using quantum walks achieves complexity $O(t)$ [7, 8]. For all of the above methods, the scaling with respect to the error ε is greater than any polynomial in $\log(1/\varepsilon)$. For example, the quantum walk approach yields scaling of $1/\sqrt{\varepsilon}$ [7, 8].

Another important task is the simulation of *time-dependent* Hamiltonians. As with constant Hamiltonians, it is possible to obtain scaling that is close to linear in time [12, 13]. The complexity then depends on the norms of the derivatives of the Hamiltonian, so if the Hamiltonian varies rapidly, then the simulation will become more costly. A method to circumvent this dependence on the derivatives is to use sampling at random times [14]. These results also scale polynomially in $1/\varepsilon$.

3 New result

Our precise result for the complexity in terms of the calls to the oracle for the Hamiltonian and additional gates is as follows.

Theorem 1. *A sparse Hamiltonian H with sparseness d specified as an oracle for the values and positions of its nonzero entries can be simulated within accuracy ε for time $t > \log(1/\varepsilon)$ with*

$$O\left(d^2\tau \frac{\log(d\tau/\varepsilon)}{\log\log(d\tau/\varepsilon)} \log^* n\right), \tag{1}$$

calls to the oracle, where $\tau := \|H\|t$, and

$$O\left(d^2\tau \log^3\!\left(\tfrac{d(\tau+\tau')}{\varepsilon}\right) \operatorname{poly}(n)\right) \tag{2}$$

additional gates, where $\tau' := \|H'\|t$ (the time-derivative of $\|H\|$, multiplied by t).

Thus we see that both the number of oracle calls and the number of additional gates scales linearly in $d^2\|H\|t$, times a factor that is polylogarithmic in the system parameters. Most significantly, the complexity scales polylogarithmically in $1/\varepsilon$, whereas previous methods scaled polynomially in $1/\varepsilon$. In addition, the complexity scales logarithmically in the norm of the derivative of H, whereas most previous techniques scale polynomially in $\|H'\|$. The additional gates are taken to be any unitary gates on at most two qubits.

4 Formal definition of Hamiltonian oracle

For the time-independent case, the input to the oracle is $x \in \{0,1\}^n$ and $k \in \{1, 2, \ldots, d\}$, and the output is $y \in \{0,1\}^n$ and α (a complex number specified to some precision), where there is a functional relationship between (x, k) and (y, α). To explain this relationship, let $i_1, \ldots, i_d \in \{0,1\}^n$ be the positions of the nonzero-entries of row x of H in some arbitrary but fixed order. Then $y = i_k$ (the position of the k-th nonzero entry of row x of H) and $\alpha = H_{x,y}$ (the value of the matrix entry of H in row x and column y). For the time-dependent case, there is an additional input: a time parameter.

5 Main ideas behind the method

The main idea is to incorporate the methodologies that have been developed for simulating continuous-time query models [10, 11] into the sparse Hamiltonian simulation context. Our key observation is that any self-inverse Hamiltonian effectively behaves as a query oracle, permitting a variant of the techniques in [10, 11] to apply (with several query Hamiltonians and a zero driving Hamiltonian). We also extend some of the results in [5] to efficiently express a sparse Hamiltonian as a linear combination of self-inverse Hamiltonians.

References

[1] R. P. Feynman, International Journal of Theoretical Physics **21**, 467 (1982).

[2] S. Lloyd, Science **273** 1073 (1996).

[3] D. Aharonov and A. Ta-Shma, *Adiabatic quantum state generation and statistical zero knowledge*, in *Proceedings of the 35th ACM Symposium on Theory of Computing, 2003* (ACM, New York, 2003), pp. 20–29; arXiv:quant-ph/0301023.

[4] A. M. Childs, Ph.D. thesis, Massachusetts Institute of Technology, 2004.

[5] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders, Commun. Math. Phys. **270**, 359–371 (2007).

[6] A. M. Childs and R. Kothari, *Simulating sparse Hamiltonians with star decompositions*, Theory of Quantum Computation, Communication, and Cryptography (TQC 2010), Lecture Notes in Computer Science **6519**, 94 (2011); arXiv:1003.3683.

[7] A. M. Childs, Commun. Math. Phys. **294**, 581 (2009); arXiv:0810.0312.

[8] D. W. Berry and A. M. Childs, Quantum Information and Computation **12**, 29 (2012).

[9] H. Chernoff, Annals of Mathematical Statistics **23**, 493 (1952).

[10] R. Cleve, D. Gottesman, M. Mosca, R. Somma, and D. Yonge-Mallo, *Efficient discrete-time simulations of continuous-time quantum query algorithms*, In *Proc. 41st ACM Symposium on Theory of Computing*, pp. 409–416 (2009).

[11] D. W. Berry, R. Cleve, and S. Gharibian, arXiv:1211.4637 (2012).

[12] N. Wiebe, D. W. Berry, P. Høyer, and B. C. Sanders, J. Phys. A: Math. Theor. **43**, 065203 (2010).

[13] N. Wiebe, D. W. Berry, P. Høyer, and B. C. Sanders, J. Phys. A: Math. Theor. **44**, 445308 (2011).

[14] D. Poulin, A. Qarry, R. D. Somma, and F. Verstraete, Phys. Rev. Lett. **106**, 170501 (2011).