Hamiltonian simulation with complexity polylogarithmic in the error

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Abstract. We present a quantum algorithm for simulating sparse Hamiltonian evolution with complexity polynomial in the logarithm of the inverse error. This is an exponential improvement over existing methods for Hamiltonian simulation. In addition, its scaling with respect to time is close to linear, and its scaling with respect to the time derivative of the Hamiltonian is logarithmic. These scalings improve upon most existing methods. Our method is to use a compressed Lie-Trotter formula, based on recent ideas for efficient discrete-time simulations of continuous-time quantum query algorithms.

Keywords: Hamiltonian, simulation, algorithm

1 Introduction

The simulation of physical quantum systems is important to understand novel physical phenomena, and is a major potential application of quantum computers. This is the original reason why Feynman proposed the concept of a quantum computer in 1982 [1]. In 1996, Lloyd [2], showed how to simulate evolution under Hamiltonians that are expressible as a sum of simple interaction Hamiltonians with scaling polynomial with respect to the number of qubits and the evolution time.

Aharonov and Ta-Shma [3] formulated a more abstract form of Hamiltonian simulation, dubbed the *sparse Hamiltonian* problem, where a generic sparse Hamiltonian is specified by an oracle for the values and positions of its nonzero matrix entries, and the goal is to simulate the evolution of a given state under this Hamiltonian. In addition to serving as a generic formulation for the problem of simulating Hamiltonian evolution, the sparse Hamiltonian problem occurs as a subproblem in some quantum algorithms [4, 5, 6]. Beginning with [3], a series of simulations were discovered [7, 8, 9, 10, 11, 12, 13] with improvements in efficiency in various parameters.

A drawback to these simulation algorithms is that their complexity is greater than polynomial in $\log(1/\varepsilon)$, where ε is the allowable error. Another drawback is that most techniques scale worse than $\widetilde{O}(t)$, where t is the time parameter. One technique provides scaling strictly linear in the time, at the expense of worse scaling in the error [9, 13]. A third drawback is that, for time-dependent Hamiltonians, the complexity depends strongly on the time-derivatives of the Hamiltonian [10, 11]. One technique avoids that dependence, at the expense of worse scaling in both the error and the time [14].

2 Summary of Results

We show how to solve the sparse Hamiltonian problem with exponentially improved error scaling. The result also matches the best previous methods for scaling with the time [9, 13] and time-derivatives of the Hamiltonian [14] up to log factors. For simplicity, we adopt a normalisation convention that $\|H\| \leq 1$. This entails no loss of generality because, if $\|H\| = \lambda$, then the problem can be rescaled, with λ absorbed into the time parameter.

Theorem 1 *Let H be a Hamiltonian with $\|H\| \leq 1$ (with no loss of generality) and sparseness d. Then evolution under H for time t can be simulated to precision ε with*

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

oracle calls and $O\big(d^2\, t\, \log^3(d\, t/\varepsilon)\, \mathrm{poly}(n)\big)$ elementary (1- and 2-qubit) gates, provided that $\varepsilon \geq \exp(-d^2 t)$.

The scaling with respect to ε is exponentially better than other known methods (that are polynomial in $1/\varepsilon$). Moreover, the scaling with respect to t is $\widetilde{O}(t)$, and better than that from Lie product formulas (which are order $t^{1+\Omega(1/\sqrt{\log t})}$). This algorithm can be adapted to the case of time-dependent Hamiltonians, attaining the same query complexity, and gate complexity

$$O\big(d^2 t \log^3(d\, t(1 + \|H'\|)/\varepsilon)\, \mathrm{poly}(n)\big)\,. \tag{2}$$

Here H' is the time derivative of H, and the norm is the maximum of the spectral norm over the time period. That is, the complexity is logarithmic in the derivative of the Hamiltonian, whereas previous methods (except [14]) were polynomial in the derivatives of the Hamiltonian.

3 Method

Our method uses the techniques in [15, 16] for relating the continuous-time query model with the discrete-time query model. That work was for a combination of a self-inverse oracle Hamiltonian and a driving Hamiltonian. Ref. [15] showed how to combine these Hamiltonians via a Lie-Trotter formula, then compress them by using ancillas and controlled operations to apply the evolution under the self-inverse Hamiltonian, then keeping only low Hamming weight components of the control qubits. This provided a simulation that is efficient in terms of the number

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of oracle calls. Then [16] showed how to compress operations on the control qubits to enable a simulation that is efficient in terms of the number of additional operations.

We build on that work to provide a method for simulation of general sparse Hamiltonians via three main ideas:

1. The sparse Hamiltonian is not self-inverse in general, so it is decomposed into a sum of self-inverse Hamiltonians with an appropriate weighting.

2. The methods in [15, 16] are generalised to apply to sums of many self-inverse Hamiltonians (as opposed to a single self-inverse query Hamiltonian).

3. The error scaling from [15, 16] is tightened to ensure that no terms are more than polynomial in $\log(1/\varepsilon)$.

For the first idea, we first use a decomposition into 1-sparse Hamiltonians [8, 12]. Next, we further decompose each 1-sparse Hamiltonian $\widetilde{H}$ into a sum of Hamiltonians whose nonzero entries all have the same absolute value. Since $\|H\| \leq 1$, for each $\widetilde{H}$, $\|\widetilde{H}\|_{\max} \leq 1$. Consider the real part of the off-diagonal entries of $\widetilde{H}$ first, which is in $[-1, +1]$. Round this value to nearest value of the form k/m, for $k \in \{-m, \ldots, +m\}$. It is then possible to approximate each $\widetilde{H}$ as $\frac{1}{m}\sum_{k=-m}^{+m} H_k$, where each H_k is 1-sparse with eigenvalues in $\{-1, 0, +1\}$. An illustrative example for $m = 2$ is

$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

These Hamiltonians can have have zero eigenvalues, but they can be eliminated along such lines as

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Similar procedures exist for the imaginary part of the off-diagonal entries (with 2×2 σ_y instead of σ_x blocks) as well as for the diagonal entries (which are 1×1 blocks).

For the second idea, the central difference is that the control operations now control which of the self-inverse Hamiltonians H_k are performed by the position of the one in the control qubits, as shown in Fig. 1. That is, the first controlled operation has k controlled by the position of the first one, and so forth. In contrast, Refs. [15, 16] used the positions of the ones to control how long the driving Hamiltonian was to be simulated for.

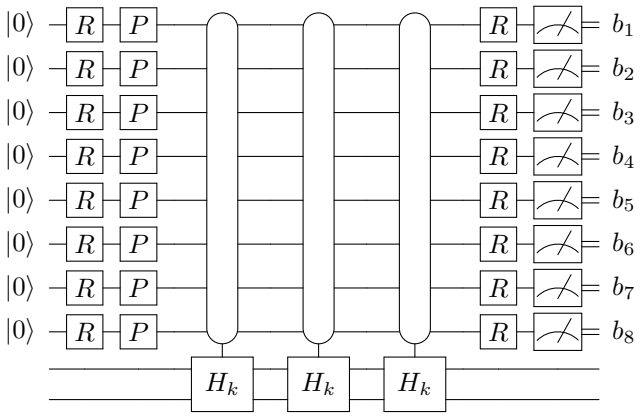

Figure 1: The Lie-Trotter formula implemented with control qubits. The self-inverse unitaries U_k are controlled by the positions of the ones in the control qubits.

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