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Algorithm for Quantum Simulation

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We summarize our algorithm for simulating Hamiltonian evolution and show that the cost of the simulation, in terms of black-box calls to the Hamiltonian oracle, is nearly linear in time and the space complexity for given sparseness is nearly constant.

Keywords: Quantum simulation, black-box calls.

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1 Introduction

Quantum computers are touted as revolutionary systems for tractably factorizing integers and solving discrete logarithms, but, in 1982, Feynman made the first proposal of a quantum computer application. He suggested that a quantum computer could efficiently simulate any local quantum system; moreover he claimed that such systems cannot in general be efficiently simulated by a (classical) Turing computer [1]. Although Feynman's intuition is legendary, the implications of his conjecture are profound, as proving a quantum computer is strictly superior to a classical computer would also prove that the complexity classes P and PSPACE are not equal.

In 1985, Deutsch generalized the Turing machine to a quantum version [2]. This introduction of a quantum computer opened the doors to studying the computation power of quantum systems in much the same way that decades of computer science research had explored the prowess and limits of classical mechanical computational devices. The theoretical side lay dormant, however, until Lloyd's analysis of Feynman's conjecture in 1996 [3]. Lloyd's approach to Feynman's conjecture was to discretize the continuous-time t evolution in terms of steps of size t/r for r the number of intervals into which the total time is divided:

$$\exp\left\{-\mathrm{i}t\sum_{j=1}^{m}\hat{H}_j\right\} = \left(\prod_{i=1}^{N}\exp\left\{-\mathrm{i}\frac{t}{r}\hat{H}_j\right\}\right)^r + \sum_{j>j'}\left[\hat{H}_j,\hat{H}_{j'}\right]\frac{t^2}{2r} + \text{Error}. \quad (1.1)$$

Lloyd demonstrated the efficiency of the protocol by showing that the cost of iterations is a polynomial function of r, m (the number of Hamiltonians that add together to yield the full Hamiltonian), and n the number of qubits over which the full Hamiltonian operates.

Subsequently Abrams and Lloyd suggested a fast algorithm for simulating many-body Fermi systems on a universal quantum computer [4]. Sørensen and Mølmer suggested a purpose-built cold-atom quantum computer to study magnetism [5]. These two papers drove further research into quantum computer research for the purpose of studying physical systems that are regarded as intractable on classical computers.

In 2003, Aharonov and Ta-Shma introduced a rigorous computer science approach to the field as they studied the problem of quantum state generation by Hamiltonian evolution and related this problem to the complexity class of statistical zero knowledge (SZK) [6]. In the course of their study, they introduced an efficient technique to simulate evolution for any sparse Hamiltonian as an oracle (black-box) problem, where "efficient" implies that the total resources, measured as the total number of qubits n_{total} and total number of gates N is a polynomial function of n, t, and $1/\epsilon$ with ϵ the tolerance for distance between the ideal state and the computed state.

2 Our Scheme

The concept behind our scheme is depicted in Fig. 2.1. The initial state Ψ_0 evolves under Hamiltonian $\hat{H}$ for time t to a final state Ψ_t in Hilbert space H. In the quantum computer, the initial state is represented by the approximation $\tilde{\Psi}_0$ in the tensor product space $H_2^{\otimes n_{\text{total}}}$, the approximated Hamiltonian by $\tilde{H}$, and the resultant state by $\tilde{\Psi}_t$. The goal is to obtain a $\tilde{\Psi}_t$ that is no further (in the sense of distance on Hilbert space) from the ideal state Ψ_0 by ϵ for any initial state and sparse Hamiltonian. In our case we assume that

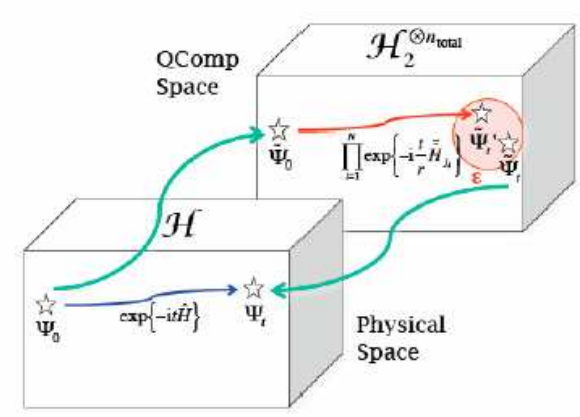

Figure 2.1: Simulating Hamiltonian evolution in a physical space on a quantum computer.

the Hamiltonian matrix $\hat{H}$ is sparse and efficiently computable: the number of non-zero terms in the matrix is at most a polynomial function of n, whereas the dimension of $\hat{H}$ is $2^n \times 2^n$, i.e. exponential in n.

We use Suzuki's method [7, 8] to decompose the unitary evolution operator into a sequence of unitary evolution operators, each generated by a one-sparse Hamiltonian $\hat{H}_j$. Beginning with the standard 'Trotter formula',

$$S_2(\lambda) = \prod_{j=1} \exp\left(\hat{H}_j \lambda/2\right) \prod_{j'=m}^{1} \exp\left(\hat{H}_j \lambda/2\right), \tag{2.1}$$

Suzuki's iterants, enumerated by index k, are

$$S_{2k}(\lambda) = \left[S_{2k-2}(p_k\lambda)\right]^2 S_{2k-2}((1-4p_k)\lambda) \left[S_{2k-2}(p_k\lambda)\right]^2 \tag{2.2}$$

for

$$p_k = \left(4 - 4^{1/(2k-1)}\right)^{-1}. \tag{2.3}$$

Suzuki then proved that

$$\left\| \exp\left(\hat{H}_j\lambda\right) - S_{2k}(\lambda) \right\| \in O\left(|\lambda|^{2k+1}\right). \tag{2.4}$$

We 'Wick-rotated' λ to it and converted Suzuki's 'order estimate' into a strictly bounded expression; then we prove the inequality (rather than an order estimate) [9]

$$\left\| \exp\left(-\mathrm{i}t \sum_{i=1}^{m} \hat{H}_i\right) - S_{2k}(-\mathrm{i}\frac{t}{r}) \right\| \leq \frac{2m5^{k-1}\left[\prod_{k'=2}^{k}(1-4p_{k'})\right] \max_j \|\hat{H}_j\| t}{(2k+1)!r^{2k}}. \tag{2.5}$$

Our theorem then states that

$$N \leq 2\frac{m5^{2k}\left(m\left[\prod_{k'=2}^{k}(1-4p_{k'})\right]\max_j\|\hat{H}_j\|t\right)^{1+1/2k}}{2\left[(2k+1)!\epsilon\right]}. \tag{2.6}$$

The exponential dependence on k is not a problem; for given time of evolution, we just optimize k to obtain

$$k_{\text{optimal}} \approx \frac{1}{2}\sqrt{\log_5\left(m\max_j\|\hat{H}_j\}t/\epsilon\right)} \tag{2.7}$$

so

$$N \leq 4m^2\max_j\|\hat{H}_j\|t\exp\left\{2\sqrt{\log_5\left(m\max_j\|\hat{H}_j\|t\right)}\right\}. \tag{2.8}$$

The number of steps thus has slightly superlinear dependence on time.

3 Coloring Graphs

We employ a graph representation of the Hamiltonian with vertices representing either row or column number and weighted edges the nonzero entries for each row or column; the weight of the edge is the value of the Hamiltonian for that row and column (because of Hermiticity, the graph can be undirected).

Using the graph representation, we develop a decomposition algorithm for the Hamiltonian into a union of degree-one graphs based on deterministic coin tossing [10, 11]. Then we devise circuits based on sequentially implementing unitary evolutions generated one-sparse Hamiltonians (represented by degree-one graphs) and concatenate them as shown in Fig. 3.1.

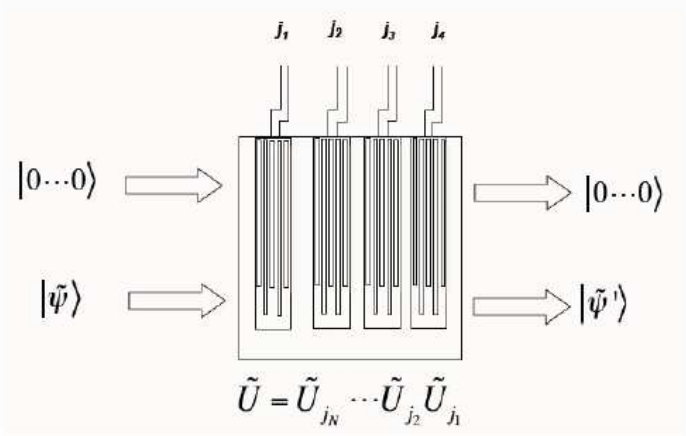

Figure 3.1: Decomposition of unitary evolution into a series of unitary gates each generated by one-sparse Hamiltonians.

4 Number of Black-Box Calls

Ultimately the question for us is not how many U-steps are required for the evolution but rather the number of black-box calls $N_{\rm bb}$. The number of black-box calls represents the full use of all resources in the quantum computer. Our result

$$N_{\rm bb} \in O\left(\frac{\log^* n d^2 5^{2k} \left[d^2 \left[\prod_{k'=2}^{k} (1 - 4p_{k'}) \right] \max_j \|\hat{H}_j\| t \right]^{1+1/2k}}{[(2k+1)!\epsilon]} \right) \tag{4.1}$$

is an order estimate and not a strict inequality. Of course this result can be optimized for given t and using $k = k_{\rm optimal}$.

5 Conclusions

We have found found an algorithm for quantum computer simulation of state evolution for a time-independent Hamiltonian. This algorithm is highly efficient: the number of black-box calls scales as $\log^* n$ for n the number of qubits for the physical system and is nearly linear in time t. More recently we have been making progress with the time-dependent case [12].

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