Hamiltonian Simulation

Quantum Computing

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Based on the notes from Ashley Montaro

April 2, 2025

Motivation

Overview

1. Introduction

Introduction: Hamiltonian Simulation

Hamiltonian

Hermitian operator acting on n qubits which corresponds physically to a system made up of n 2-level subsystems.

Schrödinger's equation

Time evolution of the state $|\psi\rangle$ of a quantum system:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

Introduction: Hamiltonian Simulation

Solution of the Schrödinger's equation (*time-independent*):

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Goal

To approximate the unitary operator:

$$U(t) = e^{-iHt}$$

Approximation in the operator (spectral) norm:

$$||A|| := \max_{|\psi\rangle \neq 0} \frac{||A|\psi\rangle||}{|||\psi\rangle||}.$$

$\tilde{U}$ approximates U within ϵ if

$$||\tilde{U} - U|| < \epsilon$$

Hamiltonian as a Pauli Matrix Product

We consider the simple case where H is proportional to a Pauli matrix on n qubits:

$$H = \alpha s_1 \otimes s_2 \otimes \cdots \otimes s_n. \tag{1}$$

The corresponding time evolution operator is:

$$e^{-itH} = e^{-it\alpha s_1 \otimes s_2 \otimes \cdots \otimes s_n}. \tag{2}$$

Challenge: H is a $2^n \times 2^n$ matrix with exponentially many parameters, but we seek a circuit of poly(n) gates.

Diagonalization of the Evolution Operator

Using the identity:

$$Ue^{-i\alpha H}U^{\dagger} = e^{-i\alpha UHU^{\dagger}}, \tag{3}$$

we diagonalize e^{-itH} with an appropriate unitary transformation:

$$e^{-itH} = (U_1 \otimes U_2 \otimes \cdots \otimes U_n)e^{-i\alpha t z_1 \otimes z_2 \otimes \cdots \otimes z_n}(U_1^{\dagger} \otimes U_2^{\dagger} \otimes \cdots \otimes U_n^{\dagger}), \tag{4}$$

where $z_i \in \{I, Z\}$.

Implementation via Quantum Circuits

The main challenge reduces to implementing:

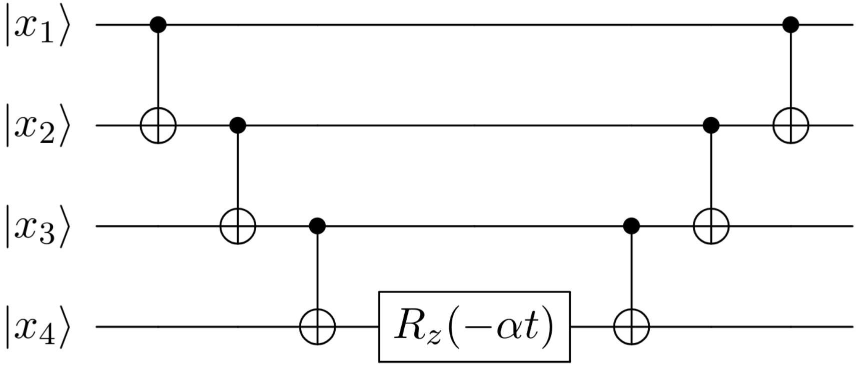
$$e^{-i\alpha t Z\otimes Z\otimes\cdots\otimes Z}. \tag{5}$$

For computational basis state x:

$$x \mapsto \begin{cases} e^{-i\alpha t}x, & \sum_i x_i \text{ even},\\ e^{i\alpha t}x, & \sum_i x_i \text{ odd}.\end{cases} \tag{6}$$

Solution: A quantum circuit using 2-qubit gates.

Quantum Circuit for $k = 4$



$$R_z(\theta) = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix}$$

Generalization to Weighted Sums of Pauli Matrices

For H as a weighted sum of commuting Pauli matrices:

$$H = \sum_{j=1}^{m} \alpha_j \sigma_{s_j}, \tag{7}$$

the evolution follows as:

$$e^{-iHt} = \prod_{j=1}^{m} e^{-i\alpha_j \sigma_{s_j} t}. \tag{8}$$

This requires $O(mn)$ quantum gates.