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Hamiltonian simulation algorithms for near-term quantum hardware

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Schrödinger equation
Lie-Trotter product formula

Problem statement

Definition

Hamiltonian simulation:
"Given a description of a Hamiltonian H, and evolution time t, some initial state $|\psi(0)\rangle$ produce the final state $|\psi(t)\rangle$ (to some error ϵ)"

- "The Hamiltonian of a system is the sum of the kinetic energies of all the particles, plus the potential energy of the particles associated with the system

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Why is this a difficult problem?

Definition

We assume that the quantum state is loaded into memory

- a classical computer can't store the state efficiently
- a classical computer cannot produce a complete description of the state

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Schrödinger equation

Definition

$H \ket{\psi(t)} = i\hbar \frac{\delta}{\delta t} \ket{\psi(t)}$

integrate both sides:

$\ket{\psi(t)} = e^{-iHt/\hbar} \ket{\psi(0)}$

break H down into potential and kinetic energy:
$\hat{V}$ (E_{pot}), $E_{kin} = p^2 \frac{1}{2m}$

$e^{\frac{-i\hat{V}t}{\hbar}}$ and $e^{\frac{-ip^2 t}{2m\hbar}}$ don't commute, $e^{-iHt/\hbar} \neq e^{\frac{-i\hat{V}t}{\hbar}} e^{\frac{-ip^2 t}{2m\hbar}}$

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Lie-Trotter product formula

Definition

$e^{A+B} = \lim_{n \to \inf}(e^{A/n}e^{B/n})^n$

- product formula: simulate the sum-terms of a Hamiltonian by simulating each one separetely for a small time slice
- $H = A + B + C$
- $U = e^{-i(A+B+C)t} = (e^{-iCt/r}e^{-iBt/r}e^{-iCt/r})^r$
- switching between kinetic and potential energy terms

we arrive at: $e^{\frac{-i\hat{H}t}{\hbar}} = \lim_{N \to \infty}(e^{\frac{-i\hat{p}^2 t}{2m\hbar N}} e^{\frac{-\hat{V}(\hat{x})t}{\hbar N}})^N$

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Split operator
Classical Approach

Definition

Split operator

Algorithm:

1. Apply a half step of the potential propagator to $\psi(0)$
2. Apply the Fourier transform: momentum basis
3. Apply a full step of the kinetic propagator on the momentum basis
4. Apply the Inverse Fourier transform: back to coordinate basis
5. Apply the second half step of the potential propagator

this algorithm results from splitting the propagator, substituting into the Schrödinger equation and projecting onto a coordinate basis $|x\rangle$

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Split operator
Classical Approach

Simulating a wavefunction

- blue line: $\langle \Psi | \Psi \rangle$
- orange line: potential energy, $\hat{V}$

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Split operator
Classical Approach

Simulating a wavefunction

- blue line: $\langle \Psi | \Psi \rangle$
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Introduction
Fermi-Hubbard Model
Sub-Circuit Model
Non-asymptotic Trotter bounds

Problem statement

Definition

Find explicit gate count for near-term simulations

- gate count of near-term quantum hardware is very limited
- algorithms need to be optimized to use as few gates as possible
- even low gate counts of 250 gates are still too costly

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Topics

- Optimal fermion encoding
- Subscircuits: programming below the circuit model
- Non-asymptotic Trotter bounds

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Introduction

Fermi-Hubbard Model

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Fermi-Hubbard Model

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Sub-Circuit Model

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Sub-Circuit Synthesis

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Error models

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Per-gate run-times
Gate decomposition cost

Run-times

Table 1 Per-gate run-times.

Fermion encoding	Trotter bounds	Standard decomposition	Sub-circuit decomposition
VC	Ref. [23], Prop. F.4.	1,243,586	977,103
	Analytic	121,478	95,447
	Numeric	5391	4236
Compact	Analytic	98,339	72,308
	Numeric	4364	3209

A comparison of the run-time $\mathcal{T}_{cost}$ for lattice size $L \times L$ with $L = 5$, overall simulation time $T = 7$ and target Trotter error $\epsilon_{target} = 0.1$, with $\Lambda = 5$ fermions and coupling strengths $|u|, |v| \le r = 1$. Obtained by minimising over product formulas up to 4th order. $\mathcal{T}_{cost}$ = circuit depth for per-gate error model. In either gate decomposition case—standard and sub-circuit—we account single-qubit rotations as a free resource as explained in the Introduction; the value of $\mathcal{T}_{cost}$ depends only on the two-qubit gates/interactions. Two-qubit unitaries are counted by unit time per gate in the per-gate error model. Here compact and VC denote the choice of fermionic encoding.

source: Hamiltonian simulation algorithms for near-term quantum hardware, Clinton et al.

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Per-gate run-times
Gate decomposition cost

Per-time run-times

Table 2 Per-time run-times.

Fermion encoding	Trotter bounds	Standard decomposition	Sub-circuit decomposition
VC	Ref. [23], Prop. F.4.	976,710	59,830
	Analytic	95,409	17,100
	Numeric	4234	1669
compact	Analytic	77,236	1686
	Numeric	3428	259

A comparison of the run-time $\mathcal{T}_{cost}$ for lattice size $L \times L$ with $L = 5$, overall simulation time $T = 7$ and target Trotter error $\epsilon_{target} = 0.1$, with $\Lambda = 5$ fermions and coupling strengths $|u|, |v| \leq r = 1$. Obtained by minimising over product formulas up to 4th order. $\mathcal{T}_{cost} = \mathcal{T}_{cost}(\mathcal{P}_p(\delta_0)^{T/\delta_0})$ for per-time error model. In either gate decomposition case—standard and sub-circuit—we account single-qubit rotations as a free resource; the value of $\mathcal{T}_{cost}$ depends only on the two-qubit gates/interactions. Two-qubit unitaries are counted by their respective pulse lengths. Here compact and VC denote the choice of fermionic encoding.

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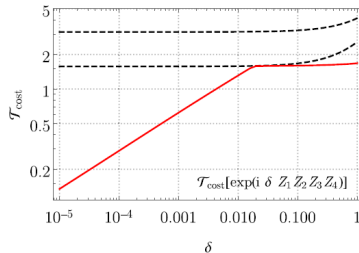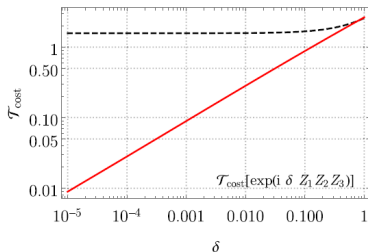
Outlook

- Further optimization needed for quantum hardware
- Tighter error bounds might be reached
- Standard circuit decomposition will stay unfeasible on real hardware for some time
- The sub-circuit model might enable some algorithm to run on NISQ hardware

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Thank you for your attention!