Hamiltonian simulation algorithms for near-term quantum hardware

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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

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

Schrödinger equation

Definition

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

integrate both sides:

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

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

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

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

Definition

Split operator

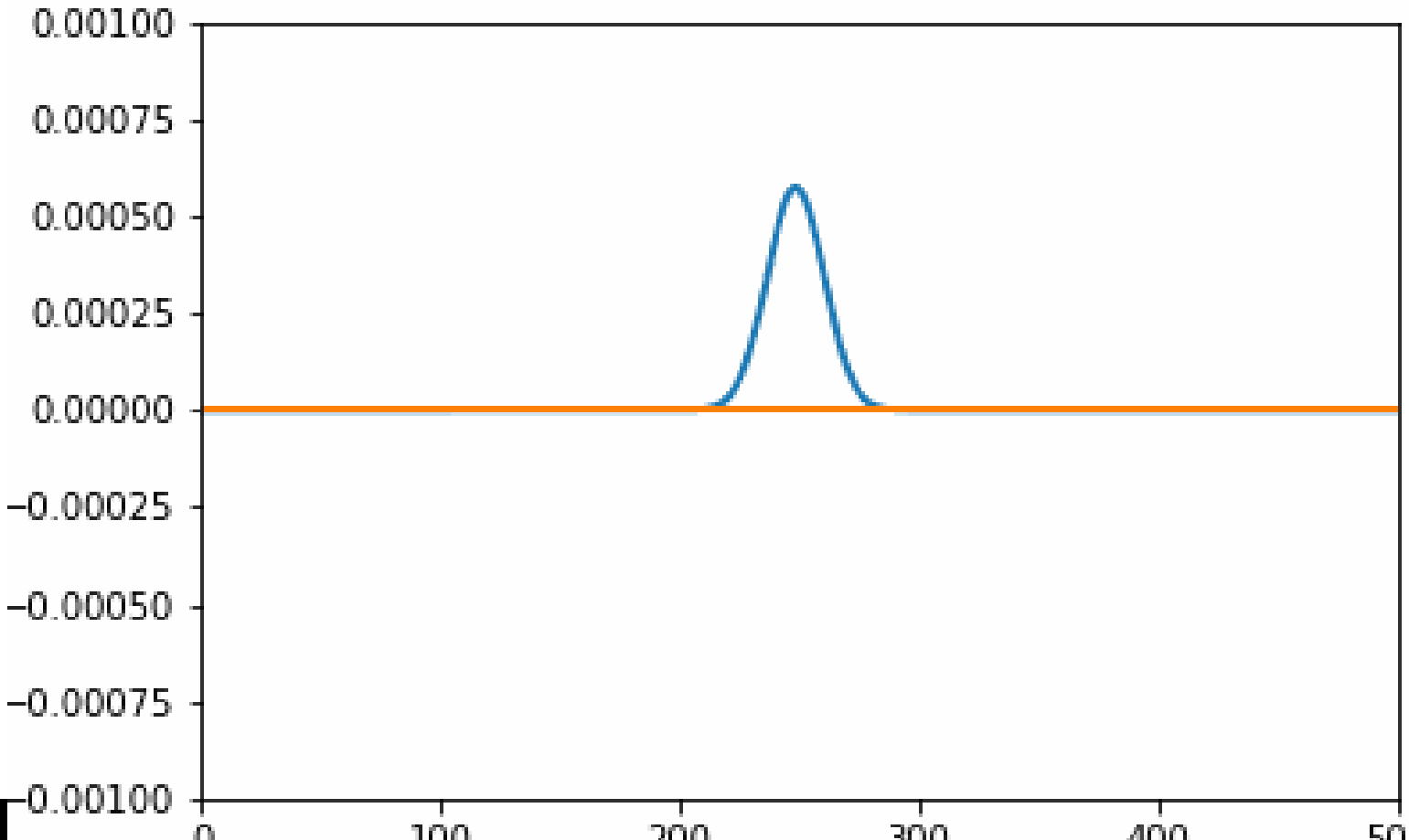
Algorithm:

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 $|x\rangle$

Simulating a wavefunction

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



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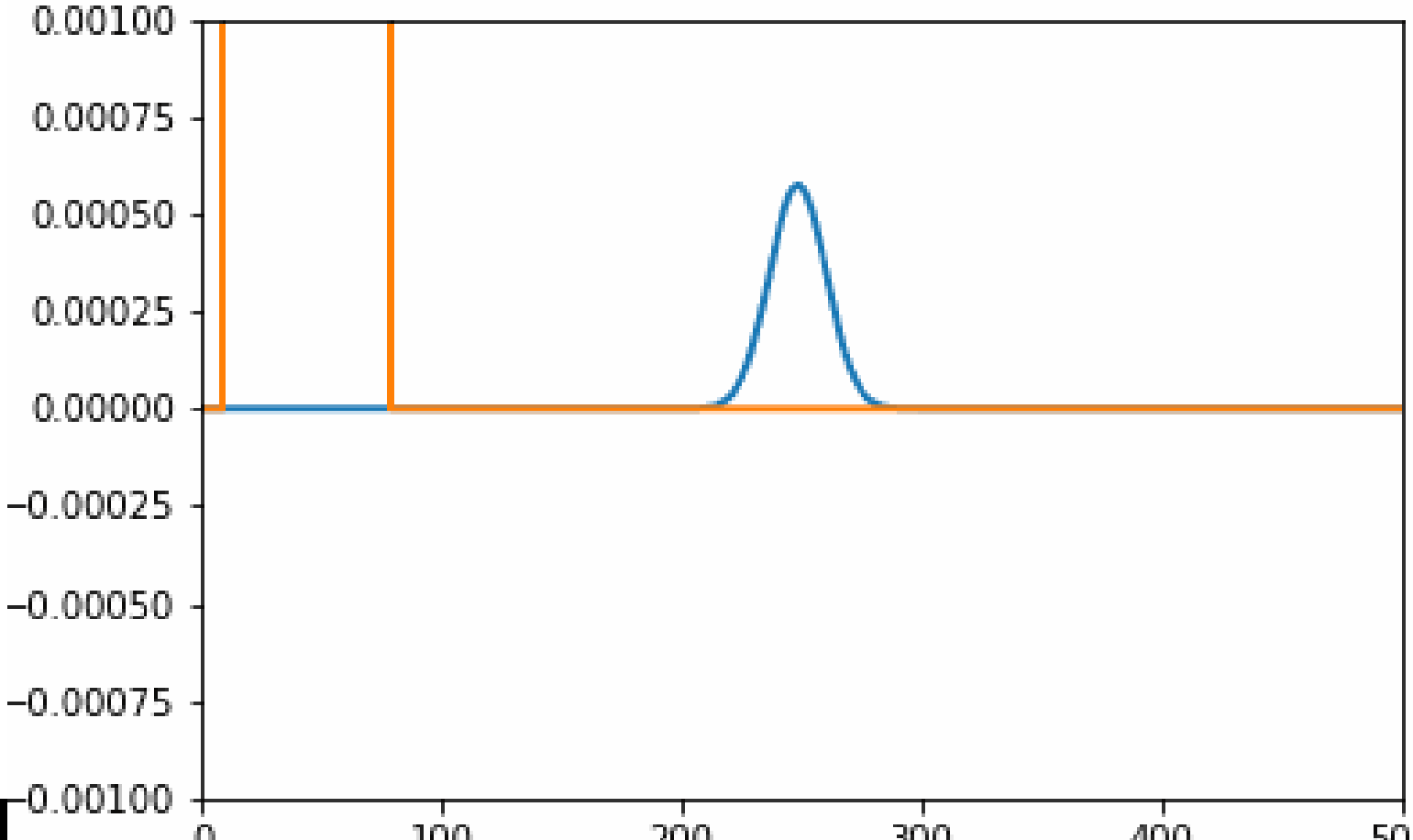


Problem statement

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

Topics

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

Fermi-Hubbard Model

Hamiltonian:
$H_{FH} = \sum_{i=1}^{N} h_{on-site}^{(i)} + \sum_{i<j,\sigma} h_{hopping}^{(i,j,\sigma)}$

- Model existed before quantum computing
- Most practical applications involve fermionic system
- Classical approaches can be used as benchmark

Sub-Circuit Model

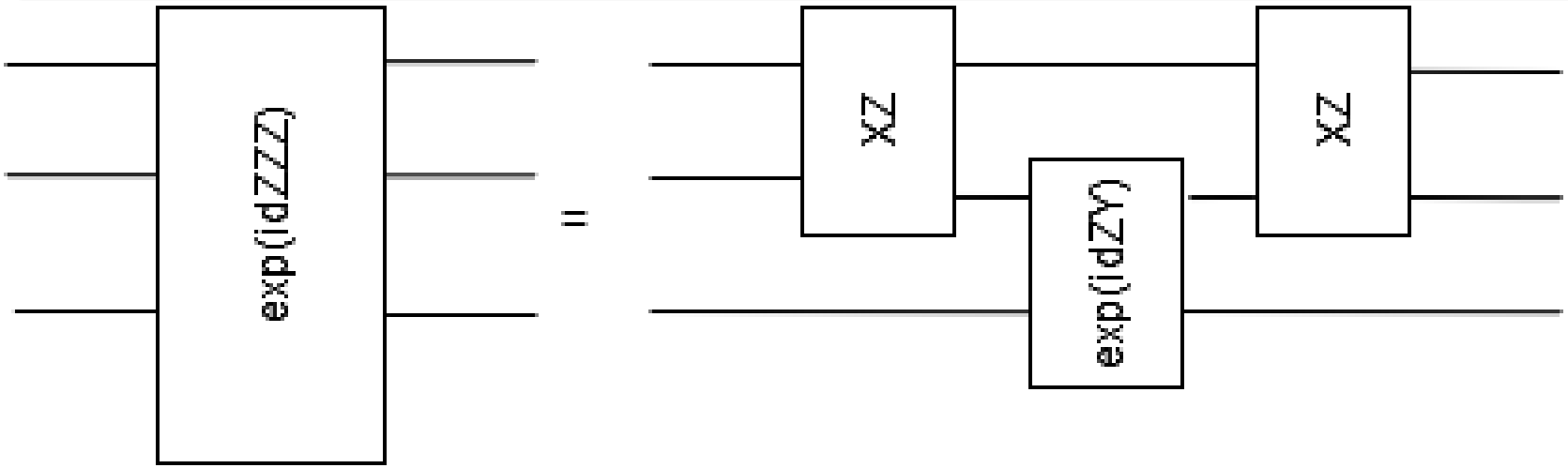
- Assumption: hardware can perform CNOT, Z, H .... gates
- Layer of abstraction: overhead
- Quantum circuit: $C = \prod_l^L U_l V_j$
- $\mathrm{U}_l = \prod_{i \in Q} u_i^l$ a layer of arbitrary single qubit unitary gates
  $\mathrm{V}_l = \prod_{ij \in \Gamma} v_{ij}(t_{ij}^l)$ a layer of non-overlapping, two-qubit gates

- two-qubit unitary gates: $v_{ij}(t) = e^{ith_{ij}}, h_{ij} = Z_i Z_j$
- $h_{ij} = \sigma_i \sigma_j$ since $\sigma_i \sigma_j = Z_i Z_j (*)$
- the cost $T_{cost}(C) = L$, L = circuit depth

Sub-Circuit Synthesis

Definition

how to decompse local Trotter steps $e^{i\delta h}$
Let $U(t) = e^{itH}, H = \frac{1}{2i}[h_1, h_2]$
$U(t) = e^{it_1 h_1} e^{it_2 h_2} e^{it_2 h_1} e^{it_1 h_2}$ (Lemma 7, supplementary)



Error models

1. Per-gate error model
2. Per-time error model

- "Error budget required to execute a circuit"
- Single-qubit gates are considered free
- Obtain tight error expression $\epsilon_p(\delta)$
- Guarantee $\epsilon_p(\delta) < \epsilon_{target}$ by inverting the expression and derive a maximum possible Trotter step $\delta_0 = \delta_0(\epsilon_{target})$

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 $\mathcal{T}_{\text{cost}}$ for lattice size $L \times L$ with $L = 5$, overall simulation time $T = 7$ and target Trotter error $\epsilon_{\text{target}} = 0.1$, with $\Lambda = 5$ fermions and coupling strengths $|u|, |v| \leq r = 1$. Obtained by minimising over product formulas up to 4th order. $\mathcal{T}_{\text{cost}}$ = 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 $\mathcal{T}_{\text{cost}}$ 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.

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 $\mathcal{T}_{\text{cost}}$ for lattice size $L \times L$ with $L = 5$, overall simulation time $T = 7$ and target Trotter error $\epsilon_{\text{target}} = 0.1$, with $\Lambda = 5$ fermions and coupling strengths $|u|, |v| \leq r = 1$. Obtained by minimising over product formulas up to 4th order. $\mathcal{T}_{\text{cost}} = \mathcal{T}_{\text{cost}}(\mathcal{P}_p(\delta_0))^{T/\delta_0}$ 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 $\mathcal{T}_{\text{cost}}$ 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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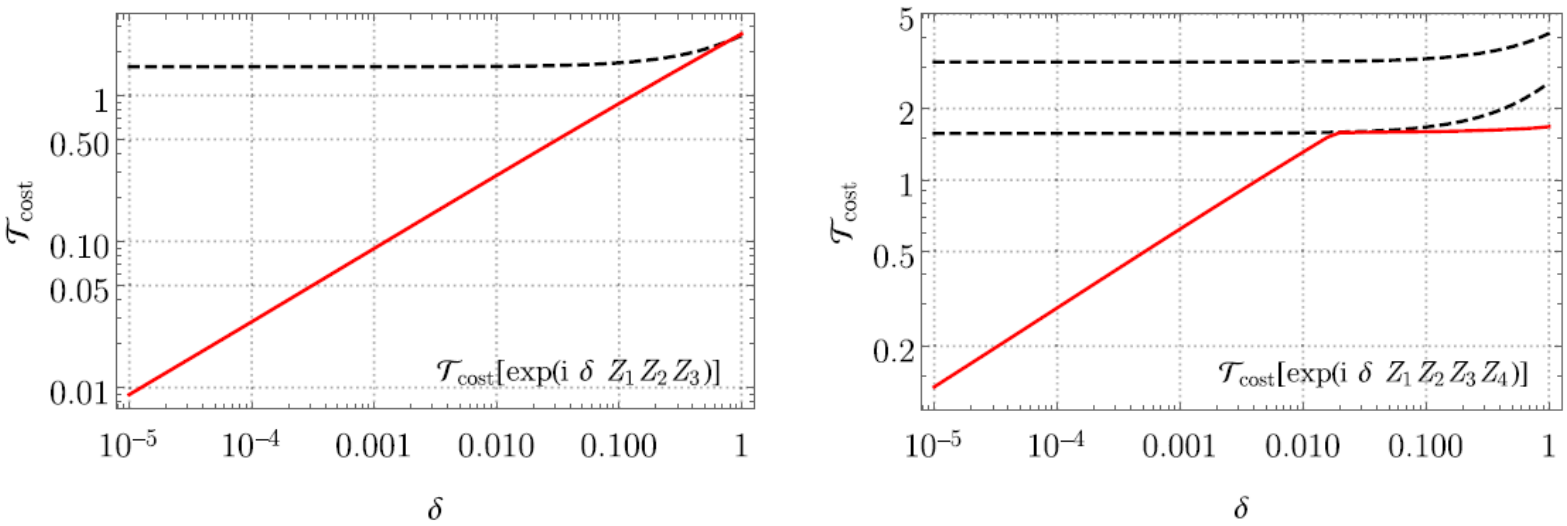
Gate decomposition cost



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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

Thank you for your attention!