On the complexity of implementing Trotter Steps

Yuan Su (Microsoft)

Joint work with
Guang Hao Low (Microsoft)
Yu Tong (Caltech)
Minh C. Tran (IBM)

arXiv:2211.09133 • PRX Quantum 4, 020323
Outline

• Background
  o Quantum computing basics
  o Analysis and implementation of Trotter-type formulas
  o Simulation of power-law Hamiltonians

• Main results

• Main techniques
  o Block encoding and low-rank diagonalization
  o Recursive method and its analysis
  o Quantum simulation in the Hamming weight-2 subspace

• Summary
State space

• The state of a single-qubit system is described by $\ell_2$-normalized vectors $|\psi\rangle = \beta_0|0\rangle + \beta_1|1\rangle \in \mathbb{C}^2$, with $\{|0\rangle, |1\rangle\}$ orthonormal and $|\beta_0|^2 + |\beta_1|^2 = 1$.

• If two subsystems are in states $|\psi\rangle$ and $|\phi\rangle$ respectively, then the joint system is in the tensor product state $|\psi\rangle \otimes |\phi\rangle$.

• More generally, an $n$-qubit quantum system can be in state

$$(\mathbb{C}^2)^\otimes n \ni \sum_{z_0,\ldots,z_{n-1}=0}^1 \beta_{z_{n-1},\ldots,z_0}|z_{n-1}\rangle \otimes \cdots \otimes |z_0\rangle$$

$$= \sum_{z_0,\ldots,z_{n-1}=0}^1 \beta_{z_{n-1},\ldots,z_0}|z_{n-1}, \ldots, z_0\rangle = \sum_{\gamma=0}^{2^{n-1}} \beta_{\gamma}|\gamma\rangle \in \mathbb{C}^{2^n}$$

with $\ell_2$-normalized coefficients.
Quantum circuit model

• Single-qubit operations are unitaries $U^\dagger U = I$ acting on $\mathbb{C}^2$:

\[
\begin{aligned}
\text{X} & := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, &
\text{Y} & := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, &
\text{Z} & := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \\
\text{Had} & := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, &
R_z(\theta) & := \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}, &
T & := \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}.
\end{aligned}
\]

• $n$-qubit operations are unitaries acting on $\mathbb{C}^{2^n}$:

\[
\begin{aligned}
\text{U} & := U \otimes V, &
\text{V} & := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \text{X} \\
\end{aligned}
\]

• In the circuit model, quantum computation is realized by a sequence of elementary quantum gates.

• **Complexity** is usually quantified by the number of gates that appear in the circuit.
Quantum simulation

Definition: Hamiltonian simulation

Given a description of Hamiltonian $H$ and evolution time $t$, approximate $e^{-itH}$ with spectral-norm error $\leq \epsilon$.

“... nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”
Toward practical quantum advantage

[Beverland, Murali, Troyer, Svore, Hoefler, Kliuchnikov, Low, Soeken, Sundaram, Vaschillo, arXiv:2211.07629]
Trotterization

• Also known as “product-formula method” or “splitting method”.

• Target system: \( H = \sum_{\gamma=1}^{\Gamma} H_{\gamma} \), where each \( H_{\gamma} \) is Hermitian and can be directly exponentiated on a quantum computer.

• Can use the first-order Lie-Trotter formula

\[
S_1(t) := e^{-it\Gamma} \cdots e^{-itH_1} = e^{-itH} + O(t^2)
\]

with Trotter error \( O(t^2) \).

• Formulas of higher order \( S_p(t) = e^{-itH} + O(t^{p+1}) \) exist.

• Long-time evolution can be simulated by repeating short steps. \#Gate = \#Step \times \#Gate/Step.
Trotter error with commutator scaling

• Trotter error has a **commutator scaling**, which implies commutator scaling of the number of Trotter steps:

\[
\text{#Step} = O \left( \|H\|_c t \left( \frac{\|H\|_c t}{\epsilon} \right)^{1/p} \right),
\]

\[
\|H\|_c := \left( \sum_{\gamma_1, \ldots, \gamma_{p+1}} \left\| [H_{\gamma_{p+1}}, \ldots, [H_{\gamma_2}, H_{\gamma_1}]] \right\| \right)^{1/(p+1)}.
\]

• One can achieve nearly linear time simulation by using a sufficiently high order formula: \(1/p = o(1)\).
Sequential Trotter steps

• Trotter steps can be implemented in a sequential manner. But the cost inevitably scales with the total Hamiltonian term number $\Gamma$. 

• For $n$-qubit 2-local Hamiltonians, 

$$\#\text{Gate/Step} \sim \Gamma \sim \binom{n}{2} \sim n^2, \quad \text{System size} \sim n.$$ 

• The gap $n^\kappa$ vs $n$ becomes larger for $\kappa$-local systems. 

• Can we perform faster Trotter steps with complexity sublinear in the term number? When and how?
Power-law Hamiltonians

**Definition: 1D Power-law Hamiltonians**

\[ H = \sum_{1 \leq j < k \leq n} H_{j,k} \],

where \( H_{j,k} \) are 2-local terms acting nontrivially only on sites \( j \) and \( k \) with norm \( \| H_{j,k} \| \leq 1/|j - k|^\alpha \) and decay exponent \( \alpha \).

- Many interaction potentials can be expressed as a power-law series
  \[ v(j,k) = \frac{c_1}{|j - k|} + \frac{c_2}{|j - k|^2} + \frac{c_3}{|j - k|^3} + \ldots \]

- This models physically relevant systems (trapped ions, Rydberg atoms, ultracold atoms/molecules, nitrogen-vacancy centers, and superconducting systems).

- In particular, we improve the electronic structure Hamiltonian simulation in real space (\( \alpha = 1 \)) over the best previous results.
Evaluating commutator scaling

- Terms in the power-law Hamiltonians are nonuniform and satisfy certain commutation relations.
- Cancelling commuting terms, we have
  \[
  \sum_{j_1,k_1,j_2,k_2,j_3,k_3,\ldots,j_{p+1},k_{p+1}} \left\|[H_{j_{p+1},k_{p+1}}, \ldots, [H_{j_3,k_3}, [H_{j_2,k_2}, H_{j_1,k_1}]]]\right\|
  \]
  \[= \sum_{j_2 \text{ or } k_2 \in \{j_1,k_1\}} \sum_{j_3 \text{ or } k_3 \in \{j_1,k_1,j_2,k_2\}} \left\|[H_{j_{p+1},k_{p+1}}, \ldots, [H_{j_3,k_3}, [H_{j_2,k_2}, H_{j_1,k_1}]]]\right\|.\]

- Furthermore, for a fixed value of \( j \),
  \[
  \sum_{j<k\leq n} \|H_j,k\| \leq \sum_{j<k\leq n} \frac{1}{|j-k|^\alpha} = \begin{cases} 
  \mathcal{O}(1), & \alpha > 1, \\
  \mathcal{O}(\log n), & \alpha = 1, \\
  \mathcal{O}(n^{1-\alpha}), & 1 > \alpha > 0.
  \end{cases}
  \]
Exponentiating Pauli strings

• In the computational basis, $ZZ$ has the action
  
  $ZZ|00\rangle = |00\rangle, \quad ZZ|01\rangle = -|01\rangle,$
  $ZZ|10\rangle = -|10\rangle, \quad ZZ|11\rangle = |11\rangle.$

• Exponentiation of Pauli strings can thus be implemented by computing parity (and changing basis):

• Parity trick holds for a general Pauli string:
Best previous result

• For $n$-qubit 1D power-law Hamiltonians,

$$
\text{#Step} \sim \begin{cases} 
  t(nt/\epsilon)^{o(1)}, & \alpha \geq 1, \\
  n^{1-\alpha}t(nt/\epsilon)^{o(1)}, & 1 > \alpha > 0.
\end{cases}
$$

• Meanwhile, #Gate/Step=$O(n^2)$ with the sequential method.

| Method     | Decay | $\alpha \geq 1$ | $1 > \alpha > 0$ |
|------------|-------|------------------|------------------|
| Sequential*| $n^2t$ | $n^{3-\alpha}t$ |

Complexity of best previous Trotterization of $n$-qubit power-law Hamiltonians with decay exponent $\alpha$ for time $t$ and accuracy $\epsilon$, neglecting $(nt/\epsilon)^{o(1)}$ factors.

* [Childs, Su, Tran, Wiebe, Zhu, arXiv:1912.08854]
Our result: Reduced Complexity

• Faster Trotter steps are possible when coefficients in the Hamiltonian have additional structural properties.

| Method             | Decay | $\alpha \geq 2$ | $2 > \alpha \geq 1$ | $1 > \alpha > 0$ |
|--------------------|-------|-----------------|----------------------|------------------|
| Sequential*        | $n^2 t$ | $n^2 t$ | $n^3 - \alpha t$ |
| Block encoding†    | $nt$   | $n^3 - \alpha t$ | $n^3 - \alpha t$ |
| Average-cost†      | —      | $n^{2 - \alpha/2} t$ | $n^{5/2 - \alpha} t$ |
| Low-rank†          | $nt$   | $nt$           | $n^{2 - \alpha} t$ |

Gate complexity comparison between our Trotterization and the best previous result for $n$-qubit power-law Hamiltonians with decay exponent $\alpha$ for time $t$ and accuracy $\epsilon$, neglecting $(nt/\epsilon)^o(1)$ factors.

* [Childs, Su, Tran, Wiebe, Zhu, arXiv:1912.08854]
† [Low, Su, Tong, Tran, On the complexity of implementing Trotter steps, arXiv:2211.09133]
Our result: Application and Limitation

• In **second quantization** in **real space**, Coulomb potential is represented as

\[ V \propto \sum_{l,m} \frac{1}{||l - m||} N_l N_m = \sum_{l,m} \frac{1}{||l - m||} \left( \frac{1 - Z_l}{2} - \frac{1 - Z_m}{2} \right). \]

• **Application**: With a slightly tighter Trotter error bound, we show that electronic structure can be simulated with gate complexity

\[
\left( \frac{\eta^{2/3} n^{4/3}}{\omega^{1/3}} + \frac{n^{5/3}}{\omega^{2/3}} \right) \frac{n^{o(1)} t^{1+o(1)}}{\epsilon^{o(1)}},
\]

with \( \eta = \# \text{electrons} \) and \( \omega = \) the computational cell volume, giving the fastest simulation of electronic structure Hamiltonians in real space.

• **Limitation**: **sequential method is optimal if Hamiltonian coefficients take arbitrary values.**
Block encoding as unitary dilation

• Problem: given matrix $H$, construct a unitary $U$ such that

$$U = \begin{bmatrix} H & * \\ * & * \end{bmatrix}. $$

• This unitary dilation is mathematically feasible if and only if $\|H\| \leq 1$: if $H = V\Sigma W^\dagger$ is SVD, then define

$$U = \begin{bmatrix} V & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} \Sigma & -\sqrt{1 - \Sigma^2} \\ \sqrt{1 - \Sigma^2} & \Sigma \end{bmatrix} \begin{bmatrix} W^\dagger & 0 \\ 0 & W^\dagger \end{bmatrix}. $$

• Assume $H = \sum_{\gamma=1}^{\Gamma} \beta_\gamma U_\gamma$, where $\beta_\gamma > 0$ and $U_\gamma$ are Hermitian unitaries such that $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U_\gamma$ can be directly implemented. Then choosing

$$\text{PREP}|0\rangle = \frac{1}{\sqrt{\|H\|_1}} \sum_{\gamma=1}^{\Gamma} \sqrt{\beta_\gamma} |\gamma\rangle, \quad \text{SEL} = \sum_{\gamma=1}^{\Gamma} |\gamma\rangle \langle \gamma| \otimes U_\gamma$$

gives

$$(\langle 0|\text{PREP}^\dagger \otimes I)\text{SEL}(\text{PREP}|0\rangle \otimes I) = \frac{H}{\|H\|_1} \text{ with } \|H\|_1 = \sum_\gamma \beta_\gamma.$$
Block encoding & quantum simulation

• One can perform quantum simulation by introducing auxiliary qubits and running quantum algorithms on larger Hilbert spaces.

• Assume $H = \sum_{\gamma=1}^{\Gamma} \beta_{\gamma} U_{\gamma}$, where $\beta_{\gamma} > 0$ and $U_{\gamma}$ are Hermitian unitaries such that $|0\rangle\langle0| \otimes I + |1\rangle\langle1| \otimes U_{\gamma}$ can be directly implemented.

• Then, perform the following circuit

\[ \text{#Step } \sim \|H\|_1 t = (\sum_{\gamma} \beta_{\gamma}) t \]

where \( \text{PREP}|0\rangle = \frac{1}{\sqrt{\|H\|_1}} \sum_{\gamma=1}^{\Gamma} \sqrt{\beta_{\gamma}} |\gamma\rangle \), \( \text{SEL} = \sum_{\gamma=1}^{\Gamma} |\gamma\rangle\langle\gamma| \otimes U_{\gamma} \).

* [Low, Chuang, arXiv:1610.06546]
Block encoding cost

• SEL has cost often **linear in the system size**:

\[
    \text{SEL} = \sum_{u,v=1}^{n} |u, v\rangle\langle u, v| \otimes X_u Y_v = \left( \sum_{u=1}^{n} |u\rangle\langle u| \otimes X_u \right) \left( \sum_{v=1}^{n} |v\rangle\langle v| \otimes Y_v \right),
\]

PREP can be improved correspondingly using structural properties of the coefficients. So **#Gate/Step ~ n**.

• However, unlike Trotter, qubitization does not have a commutator scaling

\[
    \#\text{Step} \sim \|H\|_1 t = \left( \sum_{\gamma} \beta_{\gamma} \right) t,
\]

which completely washes out the improvements from PREP and SEL for power-law interactions.
Low-rank diagonalization

• For a Hamiltonian with commuting terms, quantum simulation can be realized using a diagonalization circuit.

• Suppose $H = \sum_{u,v} \beta_{u,v} Z_u Z_v$ and the coefficient tensor has a singular value decomposition with rank $\rho$

$$\beta_{u,v} = \sum_{s=1}^{\rho} \mu_{u,s} \sigma_s \nu_{v,s}.$$ 

• Then we can simply compute the diagonal phase factors

$$e^{-itH} |z_n, \ldots, z_1\rangle = e^{-it\sum_{s=1}^{\rho} \sigma_s (\sum_{u} \mu_{u,s}(-1)^{z_u})(\sum_{v} \nu_{v,s}(-1)^{z_v})} |z_n, \ldots, z_1\rangle$$

with cost $\sim \rho n$ depending on the rank.

• However, the coefficient tensor of a general power-law Hamiltonian does not have low rank.
Recursion & the master theorem

• Solve a problem of size $n$ by solving $m$ subproblems, each of size $n/m$, and combining the answers.

• The complexity of recursion can be obtained from the master theorem:

$$
cost_{rec}(n) = m \cdot cost_{rec}\left(\frac{n}{m}\right) + cost(n)
$$

$$
\downarrow
$$

$$
cost_{rec}(n) = \mathcal{O}(cost(n) \log(n) + n)
$$

* [CLRS, Introduction to Algorithms '22] [Neapolitan, Foundations of Algorithms '14]
Recursive block encoding

- With a suitable recursion, the number of qubitization steps regains the commutator scaling of Trotterization.

- This can be further improved for small $\alpha$ by simulating commuting terms with an average combination cost.
Analysis of Taylor approximation

- Power function $f(x, y) = \frac{1}{||x-y||^\alpha}$ can be uniformly Taylor approximated, with error determined by size and distance of the regions $f$ acts on.

- Specifically, truncating the Taylor series of $d$-dimensional power functions at order $m$ gives* 

\[
\text{error: } \|f - \tilde{f}\|_{\max, x \times y} = O\left(\left(\frac{c \text{Diam}(X)}{\text{Dist}(X, Y)}\right)^m\right), \quad \text{rank: } \rho = O(m^d),
\]

where constant $c > 1/2$ can be chosen arbitrarily close to $1/2$.

* [Hackbusch, Hierarchical Matrices: Algorithms and Analysis '15, Theorem 4.22]
Recursive low-rank method

- Using the division-by-half strategy, we have

| Dimensions | $d = 1$ | $d = 2$ | $d = 3$ |
|------------|--------|--------|--------|
| $\frac{c \text{ Diam}(X)}{\text{Dist}(X, Y)}$ | $\frac{1}{2} = 0.5$ | $\frac{\sqrt{2}}{2} = 0.707 \ldots$ | $\frac{\sqrt{3}}{2} = 0.866 \ldots$ |

Thus, the Taylor error decays exponentially with the truncate order $m$. 

© Microsoft 2023

On the complexity of implementing Trotter steps
Simulation in Hamming weight-2 subspace

• If coefficients of a 2-local Hamiltonian have no specific structure, then one needs $\Omega(n^2)$ gates to simulate with $\epsilon = \Omega(1/poly(n))$ for $t = \Omega(\epsilon)$.

• We give a gate-efficient reduction: performing diagonal unitaries can be accomplished by simulating 2-local commuting Hamiltonians in the Hamming weight-2 subspace.

• Lower bound then follows from a volume-comparison technique.*

*Knill, arXiv:quant-ph/9508006
Summary

• We develop recursive methods to perform Trotter steps using structures of Hamiltonian coefficients, going beyond the sequential approach.

• \#Gate/Step is sublinear in the Hamiltonian term number, while \#Step still maintains the commutator scaling.

• The new result gives the fastest quantum simulation of second-quantized electronic structure Hamiltonians in real space. Further studies on first-quantized quantum simulation could be interesting.

• However, Trotter steps are hard to asymptotically improve if Hamiltonian coefficients are arbitrarily chosen.

• It could be fruitful to further optimize Trotter circuits and error bounds, or to find applications of product formulas beyond quantum simulation.
Learn more

“On the complexity of implementing Trotter Steps”
arXiv:2211.09133 • PRX Quantum 4, 020323

Register for the Azure Quantum Elements preview
aka.ms/quantum-elements

Watch the Quantum Innovator Webinar series
aka.ms/azure-quantum-innovators