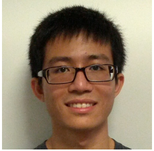
A Theory of Trotter Error

Yuan Su
University of Maryland



Andrew M. Childs
Maryland

Minh C. Tran
Maryland

Nathan Wiebe
Washington

Shuchen Zhu
Georgetown

arXiv:1901.00564/PRL **arXiv:1912.08854**

Quantum simulation

- Dynamics of a quantum system are given by its Hamiltonian $\mathscr{H}(t)$ according to the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{U}(t) = -i\mathscr{H}(t)\mathscr{U}(t), \qquad \mathscr{U}(0) = I.$$

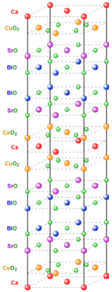
- We formally write the solution $\mathscr{U}(t) = \exp_{\mathcal{T}}\left(-i\int_0^t \mathrm{d}\tau\,\mathscr{H}(\tau)\right)$. When $\mathscr{H}(t) \equiv H$ is time-independent, we have closed-form solution $\mathscr{U}(t) = e^{-itH}$.

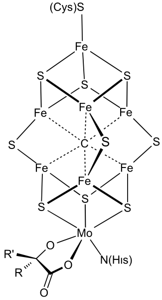
Quantum simulation problem

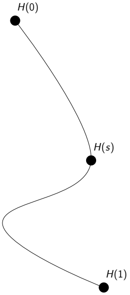
Given a description of the Hamiltonian H and evolution time t, perform e^{-itH} up to some error ϵ (in spectral norm):

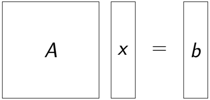
$$\left\| U - e^{-itH} \right\| \leq \epsilon.$$

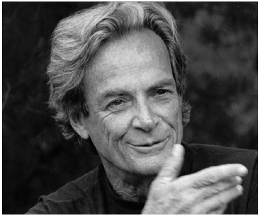
Reasons to study quantum simulation











"...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."

— Richard Feynman

Product formulas

- Also known as Trotterization or the splitting method.
- Target system: $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$, where each H_γ is Hermitian and can be exponentiated with cost $\mathcal{O}(1)$.
- Can use the first-order Lie-Trotter formula[1]

$$\mathscr{S}_1(t) := e^{-itH_\Gamma} \cdots e^{-itH_1} = e^{-itH} + O(t^2)$$

  with **Trotter error** $O(t^2)$.
- To simulate for a large t, divide the evolution into r **Trotter steps** and simulate each step with error at most ϵ/r.
- Choose the **Trotter number** r to be sufficiently large so that the entire simulation has error at most ϵ.

[1] [Lloyd 96]

Higher-order product formulas

- A general pth-order product formula takes the form

$$\mathscr{S}_p(t) := \prod_{\upsilon=1}^{\Upsilon} \prod_{\gamma=1}^{\Gamma} e^{-ita_{(\upsilon,\gamma)} H_{\pi_\upsilon(\gamma)}} = e^{-itH} + O\left(t^{p+1}\right).$$

Higher-order Suzuki formulas[2]

The $(2k)$th-order Suzuki formula $\mathscr{S}_{2k}(t) = e^{-itH} + O(t^{2k+1})$ is defined recursively by

$$\mathscr{S}_2(t) := e^{-i\frac{t}{2}H_1} \cdots e^{-i\frac{t}{2}H_\Gamma} e^{-i\frac{t}{2}H_\Gamma} \cdots e^{-i\frac{t}{2}H_1},$$
$$\mathscr{S}_{2k}(t) := \mathscr{S}_{2k-2}(u_k t)^2 \, \mathscr{S}_{2k-2}((1-4u_k)t) \, \mathscr{S}_{2k-2}(u_k t)^2,$$

where $u_k := 1/(4 - 4^{1/(2k-1)})$.

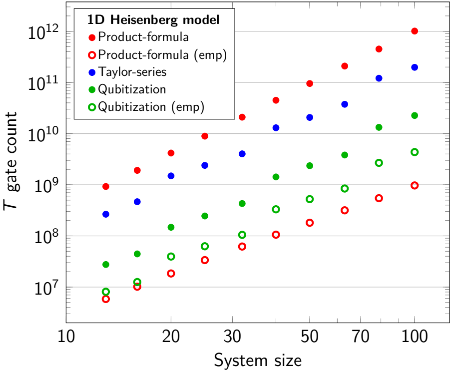
[2] [Suzuki 92]

Other simulation algorithms

- Recent algorithms have improved asymptotic performance as a function of t and ϵ over the product-formula approach...

Other simulation algorithms

- Recent algorithms have improved asymptotic performance as a function of t and ϵ over the product-formula approach...
- **... but the empirical performance of product formulas can be significantly better.**[3]

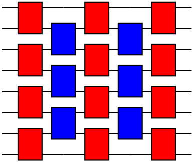


[3] [Childs, Maslov, Nam, Ross, Su 18]

Reasons to study product formulas

- The product-formula algorithm is ancilla-free and is arguably the simplest approach to quantum simulation.
- Product formulas can use Hamiltonian commutativity to give surprisingly efficient simulation in practice.
- Product formulas can preserve locality of the simulated system, which can be used to reduce the simulation cost.

$\Longleftrightarrow$



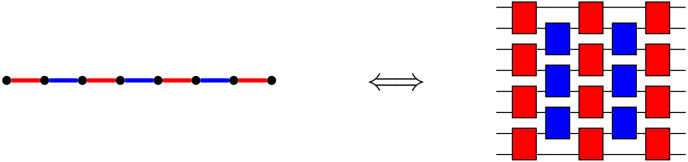
- Other applications: classical simulation of quantum systems, numerical analysis...

Reasons to study product formulas

- The product-formula algorithm is ancilla-free and is arguably the simplest approach to quantum simulation.

- **Product formulas can use Hamiltonian commutativity to give surprisingly efficient simulation in practice.**

- Product formulas can preserve locality of the simulated system, which can be used to reduce the simulation cost.



- Other applications: classical simulation of quantum systems, numerical analysis...

Previous analyses of Trotter error

- For sufficiently small t, Trotter error can be represented exactly by the Baker–Campbell–Hausdorff formula:

$$e^{-itB}e^{-itA} = e^{-it(A+B)-\frac{t^2}{2}[B,A]+i\frac{t^3}{12}[B,[B,A]]-i\frac{t^3}{12}[A,[B,A]]+\cdots}$$

- Truncating the BCH expansion ignores significant, potentially dominant contributions of Trotter error.[4]

- Using tail bounds does not exploit the commutativity of Hamiltonian summands.[5]

- Infinite-series expansion is only advantageous for systems with Lie-algebraic structure.[6]

[4] [Wecker, Bauer, Clark, Hastings, Troyer 14]
[5] [Berry, Ahokas, Cleve, Sanders 07], [Bravyi, Gosset 17]
[6] [Somma 16]

Analysis of the first-order formula

- For Hamiltonian $H = A + B$ and $t \geq 0$, the first-order formula $\mathscr{S}_1(t) = e^{-itB}e^{-itA}$ satisfies the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}_1(t) = -iH\mathscr{S}_1(t) + e^{-itB}\Big(e^{itB}iAe^{-itB} - iA\Big)e^{-itA}$$

with initial condition $\mathscr{S}_1(0) = I$.

- Using the variation-of-parameters formula,

$$\mathscr{S}_1(t) = e^{-itH} + \int_0^t \mathrm{d}\tau_1\ e^{-i(t-\tau_1)H}e^{-i\tau_1 B}\Big(e^{i\tau_1 B}iAe^{-i\tau_1 B} - iA\Big)e^{-i\tau_1 A}.$$

- We further have

$$e^{i\tau_1 B}iAe^{-i\tau_1 B} - iA = \int_0^{\tau_1}\mathrm{d}\tau_2\ e^{i\tau_2 B}\Big[iB, iA\Big]e^{-i\tau_2 B}.$$

Analysis of the first-order formula

- Altogether, we have the integral representation

$$\mathscr{S}_1(t) - e^{-itH} = \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \; e^{-i(t-\tau_1)H} e^{-i\tau_1 B} e^{i\tau_2 B} \left[iB, iA \right] e^{-i\tau_2 B} e^{-i\tau_1 A}$$

  and the error bound

$$\left\| \mathscr{S}_1(t) - e^{-itH} \right\| \le \frac{t^2}{2} \left\| \left[B, A \right] \right\|.$$

  A multi-term Hamiltonian $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ can be handled by bootstrapping the above bound.

- A similar bound holds for the second-order formula.

- Generalization to arbitrary higher-order formulas was previously unknown.

Trotter error with commutator scaling

Trotter error with commutator scaling

A pth-order product formula $\mathscr{S}_p(t)$ can approximate the evolution of Hermitian $H=\sum_{\gamma=1}^{\Gamma} H_\gamma$ for $t \geq 0$ with Trotter error

$$\left\| \mathscr{S}_p(t) - e^{-itH} \right\| = \mathcal{O}\left(\widetilde{\alpha}_{\text{comm}} t^{p+1}\right),$$

where $\widetilde{\alpha}_{\text{comm}} := \sum_{\gamma_1,\gamma_2,\dots,\gamma_{p+1}} \left\| \left[H_{\gamma_{p+1}}, \cdots \left[H_{\gamma_2}, H_{\gamma_1}\right]\right] \right\|$.

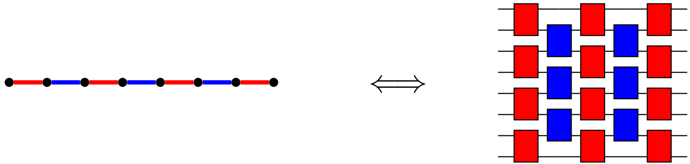
- Need $\mathcal{O}\left(\Gamma \widetilde{\alpha}_{\text{comm}}^{1/p} t^{1+1/p}\right)$ gates to achieve constant accuracy.
- Asymptotic complexity is independent of how the Hamiltonian summands are ordered.
- Related bounds exist for multiplicative error and imaginary-time evolution.

Nearest-neighbor lattice Hamiltonian

1D Nearest-neighbor lattice Hamiltonian

$H = \sum_{j=1}^{n-1} H_{j,j+1}$, where $H_{j,j+1}$ acts only on qubits j and $j+1$.

- Models many important physical systems in condensed matter physics, nuclear physics, and quantum field theory.
- Previously claimed without rigorous justification that product formulas have gate complexity $(nt)^{1+o(1)}$.[7]



[7] [Jordan, Lee, Preskill 12]

Nearest-neighbor lattice Hamiltonian

- For nearest-neighbor interactions, we can use locality to simplify $\widetilde{\alpha}_{\mathsf{comm}}$, giving

$$\widetilde{\alpha}_{\mathsf{comm}} = \sum_{\gamma_1, \gamma_2, \dots, \gamma_{p+1}} \left\| \left[H_{\gamma_{p+1}}, \cdots \left[H_{\gamma_2}, H_{\gamma_1} \right] \right] \right\| = \mathcal{O}\left(n \right).$$

- **We thus proved the Jordan-Lee-Preskill claim,** giving a simple lattice simulation with nearly optimal gate complexity.[8]

[8][Haah, Hastings, Kothari, Low 18]

Electronic structure Hamiltonian

Second-quantized plane-wave electronic structure

$$H = \underbrace{\frac{1}{2n}\sum_{j,k,\nu}\kappa_\nu^2\cos[\kappa_\nu\cdot r_{k-j}]A_j^\dagger A_k}_{T} - \underbrace{\frac{4\pi}{\omega}\sum_{j,\iota,\nu\neq 0}\frac{\zeta_\iota\cos[\kappa_\nu\cdot(\widetilde{r}_\iota - r_j)]}{\kappa_\nu^2}N_j}_{U} + \underbrace{\frac{2\pi}{\omega}\sum_{\substack{j\neq k\\ \nu\neq 0}}\frac{\cos[\kappa_\nu\cdot r_{j-k}]}{\kappa_\nu^2}N_jN_k}_{V}.$$

- An efficient simulation can help design and engineer new pharmaceuticals, catalysts and materials.
- To simulate n spin orbitals for time t, the best previous approach is the interaction-picture method[9] with complexity $\widetilde{\mathcal{O}}(n^2t)$ (and a likely large prefactor).

[9] [Low, Wiebe 18]

Electronic structure Hamiltonian

- Using fermionic Fourier transform, we can diagonalize the kinetic term in the plane-wave basis

$$\frac{1}{2n}\sum_{j,k,\nu}\kappa_\nu^2\cos[\kappa_\nu\cdot r_{k-j}]A_j^\dagger A_k=\mathsf{FFFT}^\dagger\left(\frac{1}{2}\sum_\nu\kappa_\nu^2N_\nu\right)\mathsf{FFFT}.$$

- Using the commutation rules of second-quantized operators, we estimate

$$\widetilde{\alpha}_{\mathrm{comm}}=\sum_{\gamma_1,\gamma_2,\dots,\gamma_{p+1}}\left\|\left[H_{\gamma_{p+1}},\cdots\left[H_{\gamma_2},H_{\gamma_1}\right]\right]\right\|=\mathcal{O}\left(n^{p+1}\right).$$

- **We thus showed that product formulas have gate complexity $n^{2+o(1)}t^{1+o(1)}$,** confirming a recent numerical study.[10]

[10] [Kivlichan, Gidney, Berry et al. 19]

k-local Hamiltonian

k-local Hamiltonian

$H = \sum_{j_1,\ldots,j_k} H_{j_1,\ldots,j_k}$, where each $H_{j_1,\ldots,j_k}$ acts only on $k = \mathcal{O}(1)$ qubits $j_1, \ldots, j_k$.

- Ubiquitous in physics.
- The best previous algorithm is the qubitization approach[11] with complexity $\widetilde{\mathcal{O}}(n^k \|H\|_1 t)$, scaling with the 1-norm

$$\|H\|_1 := \sum_{j_1,\ldots,j_k} \|H_{j_1,\ldots,j_k}\|.$$

[11] [Low, Chuang 19]

k-local Hamiltonian

- Using locality to simplify $\widetilde{\alpha}_{\text{comm}}$, we obtain

$$\widetilde{\alpha}_{\text{comm}} = \sum_{\gamma_1,\gamma_2,\ldots,\gamma_{p+1}} \left\| \left[H_{\gamma_{p+1}}, \cdots \left[H_{\gamma_2}, H_{\gamma_1} \right] \right] \right\| = \mathcal{O}\left(\left\| H \right\|_1^p \left\| H \right\|_1 \right),$$

where

$$\left\| H \right\|_1 := \max_l \max_{j_l} \sum_{j_1,\ldots,j_{l-1},j_{l+1},\ldots,j_k} \left\| H_{j_1,\ldots,j_k} \right\|.$$

- **We thus gave a simulation algorithm with complexity $n^k \left\| H \right\|_1 \left\| H \right\|_1^{o(1)} t^{1+o(1)}$** scaling with the induced 1-norm.

- We have the norm inequality

$$\left\| H \right\|_1 := \max_l \max_{j_l} \sum_{j_1,\ldots,j_{l-1},j_{l+1},\ldots,j_k} \left\| H_{j_1,\ldots,j_k} \right\| \leq \left\| H \right\|_1 := \sum_{j_1,\ldots,j_k} \left\| H_{j_1,\ldots,j_k} \right\|$$

and the gap can be significant for many k-local Hamiltonians.

Rapidly decaying power-law Hamiltonian

Rapidly decaying power-law Hamiltonian

$H = \sum_{\vec{i},\vec{j}} H_{\vec{i},\vec{j}}$, where $H_{\vec{i},\vec{j}}$ acts only on qubits $\vec{i}, \vec{j} \in \Lambda \subset \mathbb{R}^d$ and

$$\left\|H_{\vec{i},\vec{j}}\right\| \leq \begin{cases} 1, & \text{if } \vec{i} = \vec{j}, \\ \frac{1}{\left\|\vec{i}-\vec{j}\right\|_2^{\alpha}}, & \text{if } \vec{i} \neq \vec{j}, \end{cases}$$

with dimension d and exponent $\alpha > 2d$.

- Examples include the dipole-dipole interactions ($\alpha = 3$) and the Van der Waals interactions ($\alpha = 6$).
- The best previous approach is an algorithm based on Lieb-Robinson bounds[12] using $\widetilde{\mathcal{O}}((nt)^{1+2d/(\alpha-d)})$ gates.

[12] [Tran, Guo et al. 19]

Rapidly decaying power-law Hamiltonian

- We truncate terms with distance larger than a cut-off $\ell = \Theta\left((nt/\epsilon)^{1/(\alpha-d)}\right)$.

- For the truncated Hamiltonian, we estimate

$$\widetilde{\alpha}_{\mathrm{comm}} = \sum_{\gamma_1,\gamma_2,\ldots,\gamma_{p+1}} \left\| \left[H_{\gamma_{p+1}}, \cdots \left[H_{\gamma_2}, H_{\gamma_1}\right]\right] \right\| = \mathcal{O}\left(n\right).$$

- **We gave a product-formula algorithm with complexity $(nt)^{1+d/(\alpha-d)+o(1)}$**, outperforming the best previous approach based on Lieb-Robinson bounds.

Clustered Hamiltonian

Clustered Hamiltonian

$H = A + B = \sum_l H_l^{(1)} + \sum_l H_l^{(2)}$, where terms in A act on qubits within a single party and terms in B act between different parties.

- Appears naturally in classical fragmentation and Quantum Mechanics/Molecular Mechanics methods for large molecules.
- Group the terms within each party in A and simulate the resulting Hamiltonian using product formulas.[13]
- **Our new result implies a hybrid simulator with runtime $2^{\mathcal{O}\left(h_B^{o(1)} t^{1+o(1)} \mathrm{cc}(g)/\epsilon^{o(1)}\right)}$** with interaction strength h_B and contraction complexity $\mathrm{cc}(g)$, improving the original result $2^{\mathcal{O}(h_B^2 t^2 \mathrm{cc}(g)/\epsilon)}$.

[13] [Peng, Harrow, Ozols, Wu 19]

Transverse field Ising model

Transverse field Ising model

$H = -\sum_{1\leq u<v\leq n} j_{u,v} Z_u Z_v - \sum_{1\leq u\leq n} h_u X_u$, where X_u, Z_u are Pauli operators acting on the uth qubit and $j_{u,v} \geq 0$, $h_u \geq 0$.

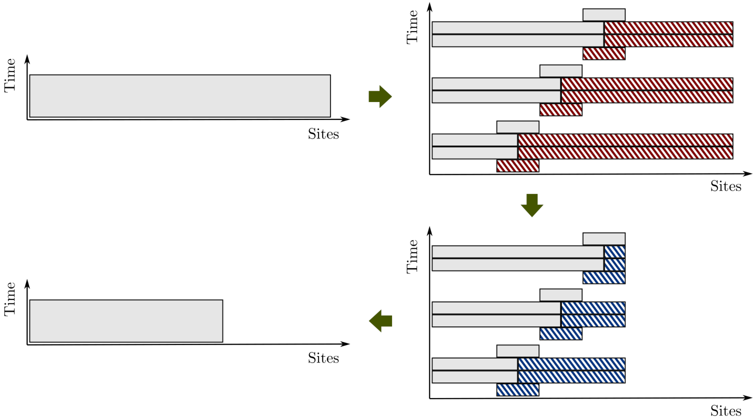
- The goal is to approximate the partition function $\mathrm{Tr}\left(e^{-H}\right)$ up to a multiplicative error.
- **We gave a Monte Carlo simulation of the transverse field Ising model with runtime $\widetilde{\mathcal{O}}\left(n^{45} j^{14} \epsilon^{-2} + n^{38} j^{21} \epsilon^{-9}\right)$**, tightening the previous result $\widetilde{\mathcal{O}}\left(n^{59} j^{21} \epsilon^{-9}\right)$ of Bravyi.[14]
- Similar improvement holds for the ferromagnetic quantum spin systems.[15]

[14] [Bravyi 15]

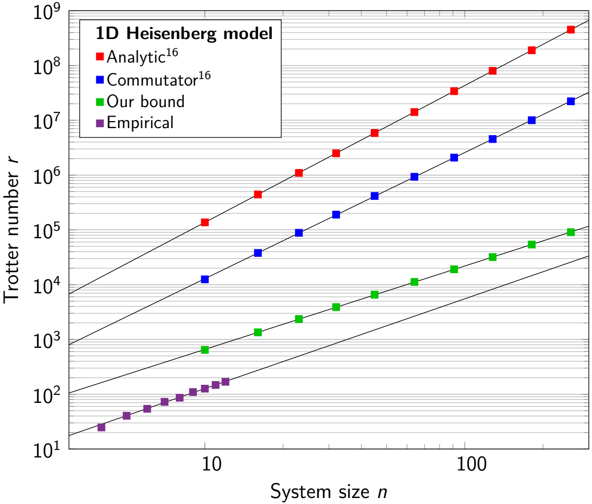
[15] [Bravyi, Gosset 17]

Simulating local observables

- We show that **local observables can be simulated with complexity independent of the system size** for power-law Hamiltonians, implying a Lieb-Robinson bound as a byproduct.



Tight prefactor



[16] [Childs, Maslov, Nam, Ross, Su 18]

A theory of Trotter error

Application	System	Best previous result	New result
Simulating quantum dynamics	Nearest-neighbor lattice	$(nt)^{1+o(1)}$ (Conjecture), $\widetilde{\mathcal{O}}(nt)$ (Lieb-Robinson bound)	$(nt)^{1+o(1)}$
	Electronic structure	$\widetilde{\mathcal{O}}\left(n^2 t\right)$ (Interaction picture)	$n^{2+o(1)} t^{1+o(1)}$
	k-local Hamiltonians	$\widetilde{\mathcal{O}}\left(n^k \\|H\\|_1 t\right)$ (Qubitization)	$n^k \vert\vert\vert H \vert\vert\vert_1 \\|H\\|_1^{o(1)} t^{1+o(1)}$
	$1/x^\alpha$ $(\alpha > 2d)$	$\widetilde{\mathcal{O}}\left((nt)^{1+2d/(\alpha-d)}\right)$ (Lieb-Robinson bound)	$(nt)^{1+d/(\alpha-d)+o(1)}$
	Clustered Hamiltonians	$2^{\mathcal{O}\left(h_B^2 t^2 \mathrm{cc}(g)/\epsilon\right)}$	$2^{\mathcal{O}\left(h_B^{o(1)} t^{1+o(1)} \mathrm{cc}(g)/\epsilon^{o(1)}\right)}$
Simulating local observables	$1/x^\alpha (\alpha > 2d)$	—	$t^{\left(1+d\frac{\alpha-d}{\alpha-2d}\right)\left(1+\frac{d}{\alpha-d}\right)+o(1)}$
Monte Carlo simulation	Transverse field Ising model	$\widetilde{\mathcal{O}}\left(n^{59} j^{21} \epsilon^{-9}\right)$	$\widetilde{\mathcal{O}}\left(n^{45} j^{14} \epsilon^{-2} + n^{38} j^{21} \epsilon^{-9}\right)$
	Quantum ferromagnets	$\widetilde{\mathcal{O}}\left(n^{115}(1+\beta^{46})/\epsilon^{25}\right)$	$\widetilde{\mathcal{O}}\left(n^{92}(1+\beta^{46})/\epsilon^{25}\right)$

- Underpinning these improvements is a theory concerning the **types**, **order conditions**, and **representations** of Trotter error.

Error types

- Suppose that we use product formula $\mathscr{S}(t)$ to approximate the evolution of H for time $t \geq 0$.
- We consider the additive, exponentiated, and multiplicative type of Trotter error

$$\mathscr{S}(t) = e^{-itH} + \int_0^t \mathrm{d}\tau \ e^{-i(t-\tau)H} \mathscr{S}(\tau) \mathscr{T}(\tau),$$

$$\mathscr{S}(t) = \exp_{\mathcal{T}}\left(-i \int_0^t \mathrm{d}\tau \big(H + \mathscr{E}(\tau)\big)\right),$$

$$\mathscr{S}(t) = e^{-itH} \exp_{\mathcal{T}}\left(-i \int_0^t \mathrm{d}\tau \ e^{i\tau H} \mathscr{E}(\tau) e^{-i\tau H}\right),$$

where $\mathscr{T}(\tau)$, $\mathscr{E}(\tau)$ consist of unitary conjugations of the form

$$e^{i\tau A_s} \cdots e^{i\tau A_2} e^{i\tau A_1} B e^{-i\tau A_1} e^{-i\tau A_2} \cdots e^{-i\tau A_s}.$$

Order conditions

- For a pth-order formula $\mathscr{S}_p(t)$, we have the following equivalent order conditions:
  - $\mathscr{S}_p(t) = e^{-itH} + O\left(t^{p+1}\right)$;
  - $\mathscr{T}_p(\tau) = O\left(\tau^{p}\right)$; and
  - $\mathscr{E}_p(\tau) = O\left(\tau^{p}\right)$.

- Order conditions can be used to cancel lower-order terms in the Taylor expansion:

$$\mathscr{F}(\tau) = O\left(\tau^{p}\right) \iff \mathscr{F}(0) = \mathscr{F}'(0) = \cdots = \mathscr{F}^{(p-1)}(0) = 0.$$

Error representations

- A unitary conjugation $e^{i\tau A_s}\cdots e^{i\tau A_2}e^{i\tau A_1}Be^{-i\tau A_1}e^{-i\tau A_2}\cdots e^{-i\tau A_s}$ has the expansion

$$C_0 + C_1\tau + \cdots + C_{p-1}\tau^{p-1} + \mathscr{C}(\tau).$$

- Time-independent operators C_0, C_1, ..., C_{p-1} can be canceled by order conditions.

- Operator-valued function $\mathscr{C}(\tau)$ is given by

$$\mathscr{C}(\tau) := \sum_{j=1}^{s} \sum_{\substack{q_1+\cdots+q_j=p \\ q_j\neq 0}} e^{i\tau A_s}\cdots e^{i\tau A_{j+1}} \cdot \int_0^\tau \mathrm{d}\tau_2\ e^{i\tau_2 A_j}\mathbf{ad}_{iA_j}^{q_j}\cdots\mathbf{ad}_{iA_1}^{q_1}(B)e^{-i\tau_2 A_j} \cdot \frac{(\tau-\tau_2)^{q_j-1}\tau^{q_1+\cdots+q_{j-1}}}{(q_j-1)!q_{j-1}!\cdots q_1!} \cdot e^{-i\tau A_{j+1}}\cdots e^{-i\tau A_s},$$

where $\mathrm{ad}_{iA_1}(B) := \left[iA_1, B\right]$.

Outlook

- simulating time-dependent Hamiltonian $\sum_{\gamma=1}^{\Gamma} \mathscr{H}_\gamma(\tau)$;
- analysis of generalized product formulas (divide-and-conquer, randomized, LCU);
- improved circuit implementation for concrete systems;
- faster numerical computation of Trotter error bounds;
- different cost metric (e.g., sub-circuit model);
- simulating low-energy state;
- simulation in the presence of noise;
- other applications...


Fractional Query
Quantum Walk
Qubitization
Taylor Series
Product Formula
A Theory of Trotter Error

Analysis of the second-order formula

- For Hamiltonian $H = A + B$ and $t \geq 0$, the second-order formula $\mathscr{S}_2(t) = e^{-i\frac{t}{2}A}e^{-itB}e^{-i\frac{t}{2}A}$ can be represented as

$$\mathscr{S}_2(t) = e^{-itH} + \int_0^t \mathrm{d}\tau_1 \; e^{-i(t-\tau_1)H}e^{-i\frac{\tau_1}{2}A}\mathscr{T}_2(\tau_1)e^{-\tau_1 B}e^{-i\frac{\tau_1}{2}A},$$

$$\mathscr{T}_2(\tau_1) = e^{-i\tau_1 B}\left(-i\frac{A}{2}\right)e^{i\tau_1 B} + i\frac{A}{2} + e^{i\frac{\tau_1}{2}A}\left(iB\right)e^{-i\frac{\tau_1}{2}A} - iB.$$

- We expand $\mathscr{T}_2(\tau_1)$ to second-order, obtaining

$$e^{-i\tau_1 B}\left(-i\frac{A}{2}\right)e^{i\tau_1 B} + i\frac{A}{2} = \left[-iB, -i\frac{A}{2}\right]\tau_1 + \int_0^{\tau_1}\mathrm{d}\tau_2\int_0^{\tau_2}\mathrm{d}\tau_3 \; e^{-i\tau_3 B}\left[-iB, \left[-iB, -i\frac{A}{2}\right]\right]e^{i\tau_3 B},$$

$$e^{i\frac{\tau_1}{2}A}\left(iB\right)e^{-i\frac{\tau_1}{2}A} - iB = \left[i\frac{A}{2}, iB\right]\tau_1 + \int_0^{\tau_1}\mathrm{d}\tau_2\int_0^{\tau_2}\mathrm{d}\tau_3 \; e^{i\frac{\tau_3}{2}A}\left[i\frac{A}{2}, \left[i\frac{A}{2}, iB\right]\right]e^{-i\frac{\tau_3}{2}A}.$$

Analysis of the second-order formula

- Altogether, we have the integral representation

$$
\begin{aligned}
&\mathscr{S}_2(t) - e^{-itH} \\
&= \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \int_0^{\tau_2} \mathrm{d}\tau_3 \; e^{-i(t-\tau_1)H} e^{-i\frac{\tau_1}{2}A} \\
&\qquad \cdot \left(e^{-i\tau_3 B}\left[-iB, \left[-iB, -i\frac{A}{2} \right]\right] e^{i\tau_3 B} + e^{i\frac{\tau_3}{2}A}\left[i\frac{A}{2}, \left[i\frac{A}{2}, iB \right]\right] e^{-i\frac{\tau_3}{2}A} \right) \\
&\qquad \cdot e^{-\tau_1 B} e^{-i\frac{\tau_1}{2}A},
\end{aligned}
$$

  and the error bound

$$
\left\| \mathscr{S}_2(t) - e^{-itH} \right\| \le \frac{t^3}{12} \left\| [B,[B,A]] \right\| + \frac{t^3}{24} \left\| [A,[A,B]] \right\| .
$$

- The general case follows by bootstrapping the above bound.

Trotter error with commutator scaling

- Consider a general pth-order product formula

$$\mathscr{S}_p(t) := \prod_{\upsilon=1}^{\Upsilon} \prod_{\gamma=1}^{\Gamma} e^{-ita_{(\upsilon,\gamma)} H_{\pi_\upsilon(\gamma)}} = e^{-itH} + O\left(t^{p+1}\right),$$

where $a_{(\upsilon,\gamma)}$ are real numbers with $|a_{(\upsilon,\gamma)}| \leq 1$.

Trotter error with commutator scaling

A pth-order formula $\mathscr{S}_p(t)$ can approximate the evolution of $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ for time $t \geq 0$ with Trotter error

$$\left\|\mathscr{S}_p(t) - e^{tH}\right\|, \left\|e^{-tH}\mathscr{S}_p(t) - I\right\| = \mathcal{O}\left(\widetilde{\alpha}_{\mathrm{comm}} t^{p+1} e^{2t\Upsilon \sum_{\gamma=1}^{\Gamma} \|H_\gamma\|}\right),$$

where $\widetilde{\alpha}_{\mathrm{comm}} := \sum_{\gamma_1,\gamma_2,\ldots,\gamma_{p+1}} \left\|\left[H_{\gamma_{p+1}}, \cdots \left[H_{\gamma_2}, H_{\gamma_1}\right]\right]\right\|$.