Nearly tight Trotterization of correlated electrons

interacting

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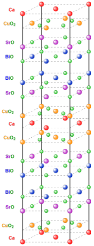
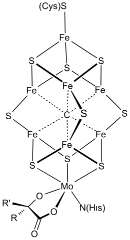
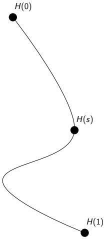
Quantum simulation

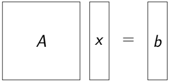
Hamiltonian simulation problem

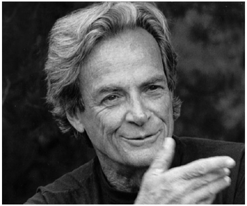
Given Hamiltonian H and time t, perform U s.t. $\left\| U - e^{-itH} \right\| \leq \epsilon$.











"... 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."

— Richard Feynman

A class of interacting electrons

Interacting electrons

$$H = T + V := \sum_{j,k=0}^{n-1} \tau_{j,k} A_j^\dagger A_k + \sum_{l,m=0}^{n-1} \nu_{l,m} N_l N_m.$$

- Jordan-Wigner encoding: on an n-qubit system,

$$A_j^\dagger = Z_0 \otimes \cdots \otimes Z_{j-1} \otimes \frac{X_j - iY_j}{2} = Z_0 \otimes \cdots \otimes Z_{j-1} \otimes |1\rangle\langle 0|_j\,,$$
$$A_k = Z_0 \otimes \cdots \otimes Z_{k-1} \otimes \frac{X_k + iY_k}{2} = Z_0 \otimes \cdots \otimes Z_{k-1} \otimes |0\rangle\langle 1|_k\,,$$
$$N_l = A_l^\dagger A_l = \frac{I - Z_l}{2} = |1\rangle\langle 1|_l\,.$$

- Represents various systems in physics and chemistry:
  - electronic-structure Hamiltonian (plane-wave basis)
  - Fermi-Hubbard model

Crash course on simulation algorithms

- LCH model: Hamiltonian $H = \sum_j H_j$, with H_j Hermitian and e^{-itH_j} implementable for arbitrary real t.
  - Trotterization (product formulas)
  - qDRIFT[1] (randomized method)
  - ...
- LCU model: Hamiltonian $H = \sum_j \alpha_j U_j$, with U_j unitary and $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U_j$ implementable.
  - Taylor-series algorithm[2]
  - Qubitization[3]
  - ...
- Interacting electrons can be simulated by many quantum algorithms, but how to further improve their runtime?

[1] [Campbell 19]
[2] [Berry, Childs, Cleve, Kothari, Somma 15]
[3] [Low, Chuang 19]

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[1][Campbell 19]
[2][Berry, Childs, Cleve, Kothari, Somma 15]
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Trotterization

- Also known as product-formula method or splitting method.
- Suffices to consider the two-term decomposition $H = T + V$, as e^{-itT} and e^{-itV} are implementable by various quantum circuits.
- Can use the first-order Lie-Trotter formula[4]

$$\mathscr{S}_1(t) := e^{-itT}e^{-itV} = e^{-itH} + O\left(t^2\right)$$

or the second-order Suzuki formula

$$\mathscr{S}_2(t) := e^{-i\frac{t}{2}V}e^{-itT}e^{-i\frac{t}{2}V} = e^{-itH} + O\left(t^3\right).$$

- Generalizations to arbitrarily high-order formula $\mathscr{S}_p(t)$ exist.[5]

[4] [Lloyd 96]
[5] [Suzuki 92]

Hamiltonian commutativity

Commutativity of fermionic operators[6]

$$\left[A_l^\dagger A_m, A_j^\dagger\right] = \begin{cases} A_l^\dagger, & j = m, \\ 0, & j \neq m, \end{cases} \qquad \left[A_l^\dagger A_m, A_k\right] = \begin{cases} -A_m, & k = l, \\ 0, & k \neq l. \end{cases}$$

- Commutator analysis existed for certain low-order formulas:

$$\mathscr{S}_1(t) - e^{-itH} = \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \; e^{-i(t-\tau_1)H} e^{-i\tau_1 T} e^{i\tau_2 T} [iT, iV] e^{-i\tau_2 T} e^{-i\tau_1 V},$$

$$\mathscr{S}_2(t) - e^{-itH} = \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \int_0^{\tau_2} \mathrm{d}\tau_3 \; e^{-i(t-\tau_1)H} e^{-i\frac{\tau_1}{2}V}$$
$$\cdot \left(e^{-i\tau_3 T} \left[-iT, \left[-iT, -i\frac{V}{2}\right]\right] e^{i\tau_3 T} + e^{i\frac{\tau_3}{2}V} \left[i\frac{V}{2}, \left[i\frac{V}{2}, iT\right]\right] e^{-i\frac{\tau_3}{2}V} \right) e^{-i\tau_1 T} e^{-i\frac{\tau_1}{2}V}.$$

- Analysis of the general case has remained elusive until recently.[7]

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[6] [Helgaker, Jørgensen, Olsen 13]
[7] [Childs, Su, Tran, Wiebe, Zhu 21]

Prior knowledge of initial state

Transition amplitude of fermionic operators

$\left|\langle\phi_\eta| \sum_{j=0}^{n-1} N_j |\psi_\eta\rangle\right| \leq \eta$ if states $|\psi_\eta\rangle$ and $|\phi_\eta\rangle$ are in the η-electron subspace $\text{span}\{|c_0, c_1, \ldots, c_{n-1}\rangle, \#\{c_j = 1\} = \eta\}$.

- Related bounds existed for simple fermionic operators:

$$|\langle\phi_\eta| T |\psi_\eta\rangle| = \left| \langle\phi_\eta| \sum_{j,k=0}^{n-1} \tau_{j,k} A_j^\dagger A_k |\psi_\eta\rangle \right| \leq \|\tau\| \eta,$$

$$|\langle\phi_\eta| V |\psi_\eta\rangle| = \left| \langle\phi_\eta| \sum_{l,m=0}^{n-1} \nu_{l,m} N_l N_m |\psi_\eta\rangle \right| \leq \|\nu\|_{\max} \eta^2.$$

- To handle the general case, insert η-electron projection Π_η and apply triangle inequality:

$$\|\Pi_\eta [T, V] \Pi_\eta\| \leq 2 \|\Pi_\eta T \Pi_\eta\| \cdot \|\Pi_\eta V \Pi_\eta\| \leq 2 \|\tau\| \|\nu\|_{\max} \eta^3.$$

Commutativity + initial-state knowledge

- So the performance of quantum simulation can be improved using either:
  - Hamiltonian commutativity (complexity depends on n, but the overall scaling is better when $\eta \approx n$);
  - initial-state knowledge (complexity depends on η, but the overall scaling is worse when $\eta \approx n$).

"But a great product isn't just a collection of features. It's how it all works together."

— Timothy Cook

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— **Quantum** Timothy Cook

Transition amplitude of Trotter error

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A pth-order formula $\mathscr{S}_p(t)$ can simulate the evolution of an n spin-orbital interacting-electronic Hamiltonian H with error

$$\left|\langle\phi_\eta\right|\left(\mathscr{S}_p(t)-e^{-itH}\right)\left|\psi_\eta\rangle\right|=\mathcal{O}\left(\left(\|\tau\|+\|\nu\|_{\max}\eta\right)^{p+1}\eta t^{p+1}\right).$$

Furthermore, if the interactions are d-sparse,

$$\left|\langle\phi_\eta\right|\left(\mathscr{S}_p(t)-e^{-itH}\right)\left|\psi_\eta\rangle\right|=\mathcal{O}\left(\left(\|\tau\|_{\max}+\|\nu\|_{\max}\right)^{p+1}d^{p+1}\eta t^{p+1}\right).$$

- The result avoids the explicit scaling with n while reducing the dependence on η, improving over previous work.[8,9]
- Analysis of Trotter error can sometimes be loose, but...

[8] [Childs, Su, Tran, Wiebe, Zhu 21]

[9] [Babbush, Wiebe, McClean, McClain, Neven, Chan 18]

Tightness

Tightness

For $s, w > 0$ and positive integer $\eta \leq \frac{n}{2}$, there exists an n spin-orbital interacting-electronic Hamiltonian with $\|\tau\| = s$ and $\|\nu\|_{\max} = w$ such that[10]

$$\Big\| \underbrace{[T, \dots [T}_{p}, V]] \Big\|_\eta = \Omega\left(s^p w \eta\right), \quad \Big\| \underbrace{[V, \dots [V}_{p}, T]] \Big\|_\eta = \Omega\left((w\eta)^p s/n\right).$$

In addition, for $u, w > 0$ and positive integer $d \leq \eta \leq \frac{n}{2}$, there exists a d-sparse n spin-orbital interacting-electronic Hamiltonian with $\|\tau\|_{\max} = u$ and $\|\nu\|_{\max} = w$ such that

$$\Big\| \underbrace{[T, \dots [T}_{p}, V]] \Big\|_\eta = \Omega\left((ud)^p wd\right), \quad \Big\| \underbrace{[V, \dots [V}_{p}, T]] \Big\|_\eta = \Omega\left((wd)^p u\right).$$

[10] $\|\cdot\|_\eta = \max_{|\psi_\eta\rangle, |\phi_\eta\rangle} |\langle\phi_\eta| \cdot |\psi_\eta\rangle|$ is the maximum transition amplitude.

Electronic structure

Second-quantized plane-wave electronic structure

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

Simulation Algorithm	n, η	$\eta = \Theta(n)$
Interaction-picture (first quantization)[11]	$\widetilde{\mathcal{O}}\left(n^{1/3}\eta^{8/3}\right)$	$\widetilde{\mathcal{O}}\left(n^3\right)$
Qubitization (first quantization)[11]	$\widetilde{\mathcal{O}}\left(n^{2/3}\eta^{4/3} + n^{1/3}\eta^{8/3}\right)$	$\widetilde{\mathcal{O}}\left(n^3\right)$
Interaction-picture (second quantization)[12]	$\widetilde{\mathcal{O}}\left(\frac{n^{8/3}}{\eta^{2/3}}\right)$	$\widetilde{\mathcal{O}}\left(n^2\right)$
Trotterization (second quantization)[13]	$\left(n^{5/3}\eta^{1/3} + n^{4/3}\eta^{5/3}\right)n^{o(1)}$	$n^{3+o(1)}$
Trotterization (second quantization)[14]	$\left(\frac{n^{7/3}}{\eta^{1/3}}\right)n^{o(1)}$	$n^{2+o(1)}$
Trotterization (second quantization)	$\boldsymbol{\left(\frac{n^{5/3}}{\eta^{2/3}} + n^{4/3}\eta^{2/3}\right)n^{o(1)}}$	$\boldsymbol{n^{2+o(1)}}$

[11] [Babbush, Berry, McClean, Neven 19]
[12] [Low, Wiebe 18]
[13] [Babbush, Wiebe, McClean, McClain, Neven, Chan 18]
[14] [Childs, Su, Tran, Wiebe, Zhu 21]

Fermi-Hubbard model

Fermi-Hubbard model

$$H = -s \sum_{\langle j,k \rangle,\sigma} \left(A_{j,\sigma}^{\dagger} A_{k,\sigma} + A_{k,\sigma}^{\dagger} A_{j,\sigma} \right) + v \sum_{j} N_{j,0} N_{j,1},$$

where $\langle j, k \rangle$ ranges over nearest-neighbor lattice sites and $\sigma \in \{0, 1\}$ labels the spin degree of freedom.

- We show that a pth-order Trotterization has gate complexity $\mathcal{O}\left(n\eta^{1/p}\right)$, improving over previous work.[15, 16]
- This improvement is not as much dramatic since the physically relevant regime is close to half filling.

[15] [Childs, Su 19]

[16] [Clinton, Bausch, Cubitt 20]

Bounding the transition amplitude

- For number-preserving operator X, bound $|\langle\phi_\eta| X |\psi_\eta\rangle|$.
- Examples:
  - $|\langle\phi_\eta| T |\psi_\eta\rangle| = \left|\langle\phi_\eta| \sum_{j,k=0}^{n-1} \tau_{j,k} A_j^\dagger A_k |\psi_\eta\rangle\right| \le \|\tau\| \eta$
  - $|\langle\phi_\eta| V |\psi_\eta\rangle| = \left|\langle\phi_\eta| \sum_{l,m=0}^{n-1} \nu_{l,m} N_l N_m |\psi_\eta\rangle\right| \le \|\nu\|_{\max} \eta^2$
- But what about more complicated fermionic operators?

$$X = \sum_{\boldsymbol{j},\boldsymbol{k}} \tau_{j_2,k_2}\delta_{k_2,j_1}\tau_{j_1,k_1} A_{j_2}^\dagger C_{2,1} B_{1,1} A_{k_1},$$

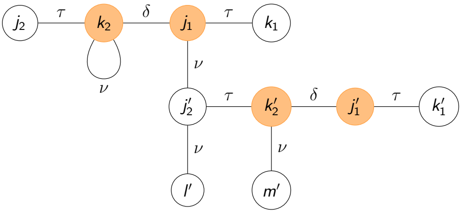
$$C_{2,1} = \nu_{k_2,k_2},$$

$$B_{1,1} = \sum_{\boldsymbol{j}',\boldsymbol{k}'} \beta_{1,2}\tau_{j_2',k_2'}\delta_{k_2',j_1'}\tau_{j_1',k_1'} A_{j_2'}^\dagger B_{2,1}' C_{2,1}' A_{k_1'},$$

$$\beta_{1,2} = \nu_{j_2',j_1},$$

$$B_{2,1}' = \sum_{l'} \nu_{l',j_2'} N_{l'},$$

$$C_{2,1}' = \sum_{m'} \nu_{k_2',m'} N_{m'}.$$



Bounding the transition amplitude

- Recursive approach: for number-preserving operator X,

$$|\langle\phi_\eta| X |\psi_\eta\rangle| = \sqrt{\langle\psi_\eta| X^\dagger |\phi_\eta\rangle \langle\phi_\eta| X |\psi_\eta\rangle} \leq \sqrt{\langle\psi_\eta| X^\dagger X |\psi_\eta\rangle}.$$

  - Contract the indices in $X^\dagger X$ by using either diagonalization or an operator Cauchy-Schwarz inequality.[17]
  - Apply a Hölder-type inequality to recursively bound $X^\dagger X$.

- Path-counting approach: for number-preserving operator X,

$$|\langle\phi_\eta| X |\psi_\eta\rangle| \leq 2\,|\langle\psi_\eta| X |\psi_\eta\rangle|\,.$$

  - Expand X, $|\psi_\eta\rangle$ and combinatorially count "paths" with nonzero contribution to the expectation.

- Full details in arXiv:2012.09194.

[17] [Otte 10]

Summary

- Improved quantum simulation by simultaneously exploiting the Hamiltonian commutativity, the sparsity of interactions, and the initial-state knowledge.

- New techniques for bounding the transition amplitude and expectation of fermionic operators.

- Simulating electronic structure in the plane-wave basis with $\left(\frac{n^{5/3}}{\eta^{2/3}} + n^{4/3}\eta^{2/3}\right) n^{o(1)}$ gates, currently the fastest in second quantization while conditionally better than first-quantized results.

- Improved simulation of the Fermi-Hubbard model.

- Concrete example Hamiltonians for which the bound is almost saturated.

Outlook

- Low-energy quantum simulation:
  - [Şahinoğlu, Somma, arXiv:2006.02660]
- Faster simulation using Hamiltonian symmetry:
  - [Tran et al., arXiv:2006.16248]
- Quantum chemistry with more compact basis:
  - [von Burg, Low et al., arXiv:2007.14460]
  - [Lee, Berry et al., arXiv:2011.03494]
- Simulation algorithms for estimating expectation values:
  - [Chen, Huang, Kueng, Tropp, arXiv:2008.11751]
  - [Faehrmann, Steudtner et al., arXiv:2101.07808]
- Simulation algorithms under different cost metric:
  - [Clinton, Bausch, Cubitt, arXiv:2003.06886]
- See Andrew's tutorial for other related work (and much more!)