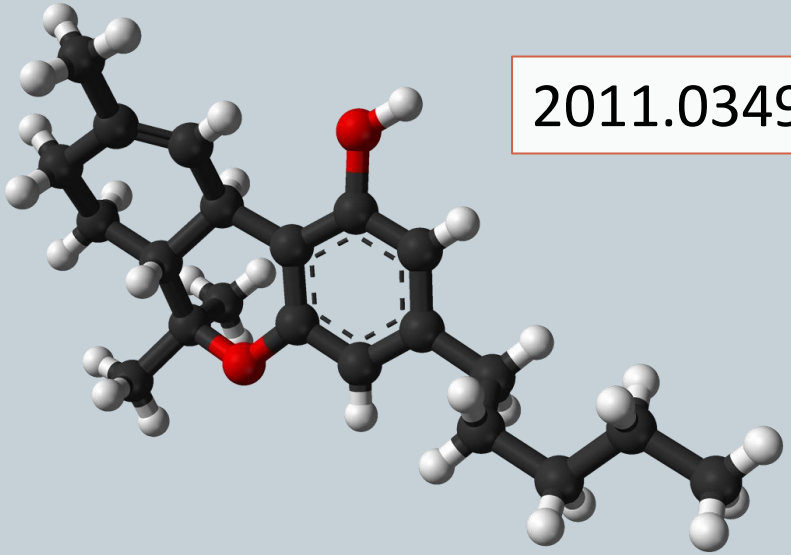
Efficient quantum computation of chemistry through tensor hypercontraction



2011.03494

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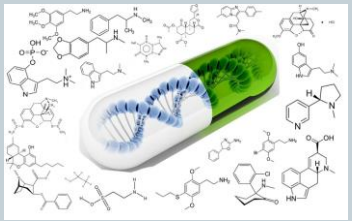
Quantum algorithms for quantum chemistry

- Quantum simulation can be used to solve extremely important problems.



Quantum algorithms for quantum chemistry

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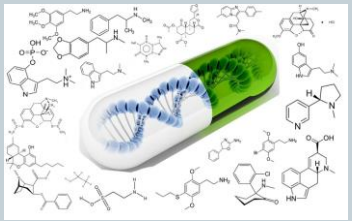
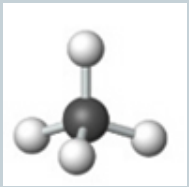
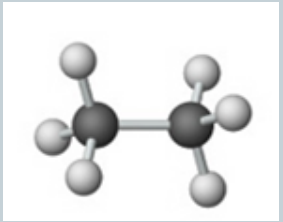


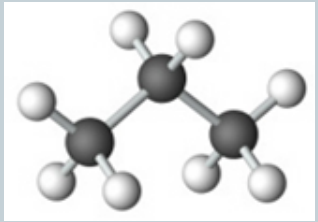
- Classical methods quickly become intractable.



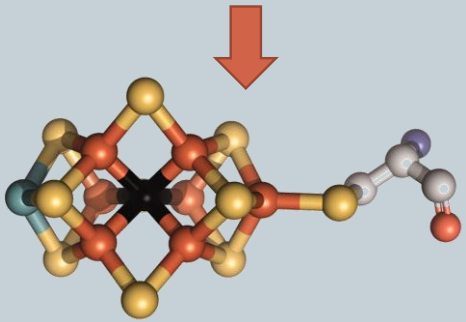
CPU seconds



CPU minutes



CPU days



FeMoco active site

Progression of complexities

Algorithm	H chain thermodynamic limit (as system grows)	H_4 continuum limit (increasing precision)
Taylor series database [1]	$\tilde{O}(N^{5.3}/\epsilon)$	$\tilde{O}(N^{7.1}/\epsilon)$
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[1] R. Babbush, D. W. Berry, I. D. Kivlichan, A. Y. Wei, P. J. Love, A. Aspuru-Guzik, New Journal of Physics **18**, 33032 (2016).
[2] E. Campbell, Physical Review Letters **123**, 070503 (2019).
[3] I. D. Kivlichan, C. E. Granade, N. Wiebe, arXiv:1907.10070 (2019).
[4] D. W. Berry, C. Gidney, M. Motta, J. McClean, R. Babbush, Quantum **3**, 208 (2019).
[5] V. von Burg, G. H. Low, T. Häner, D. S. Steiger, M. Reiher, M. Roetteler, M. Troyer, arXiv:2007.14460 (2020).
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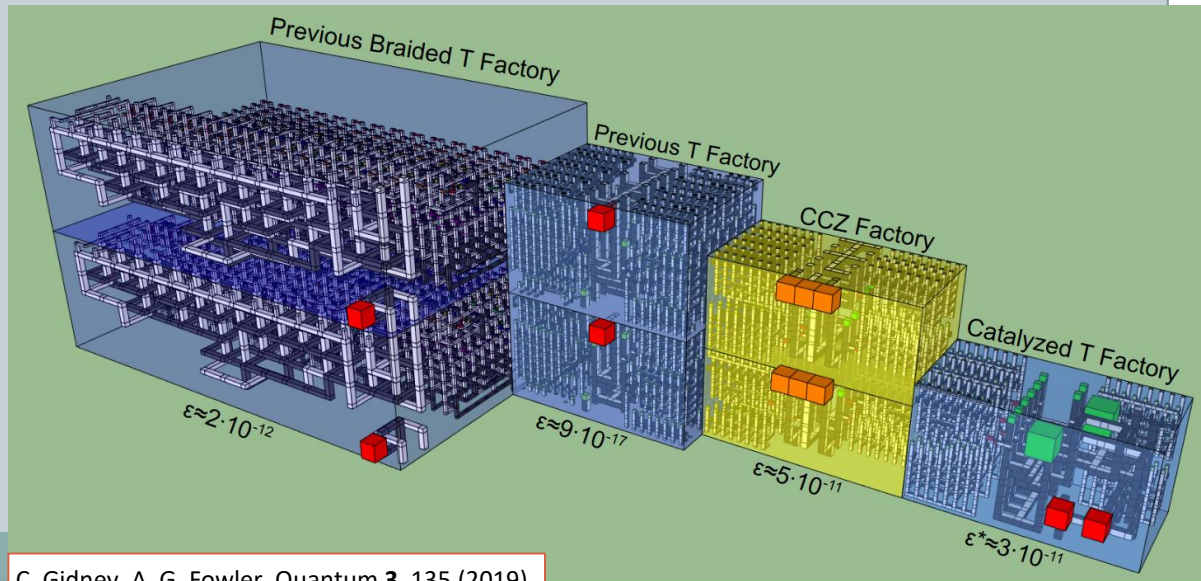
Non-Clifford gates

- Clifford gates like X and CNOT are easy in surface code.
- Non-Clifford gates like T and Toffoli* are harder.
- Can distill magic states for Toffolis directly.
- We count Toffoli gates.

*Toffolis are controlled CNOTs



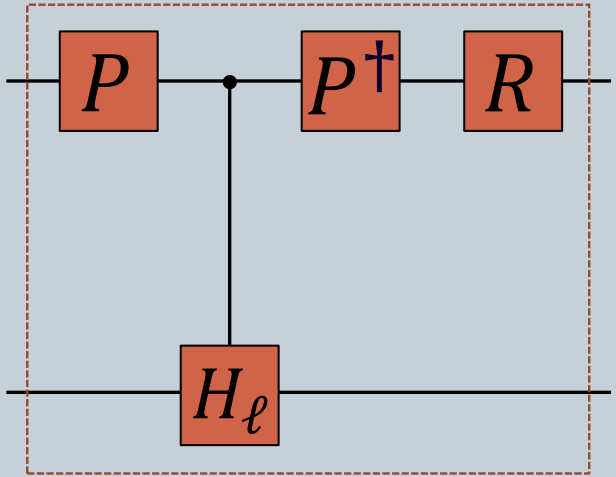
C. Gidney, A. G. Fowler, Quantum **3**, 135 (2019).

*: conditioned on no previous errors

Qubitisation

$$H = \sum_{\ell} w_\ell H_\ell$$

$W =$



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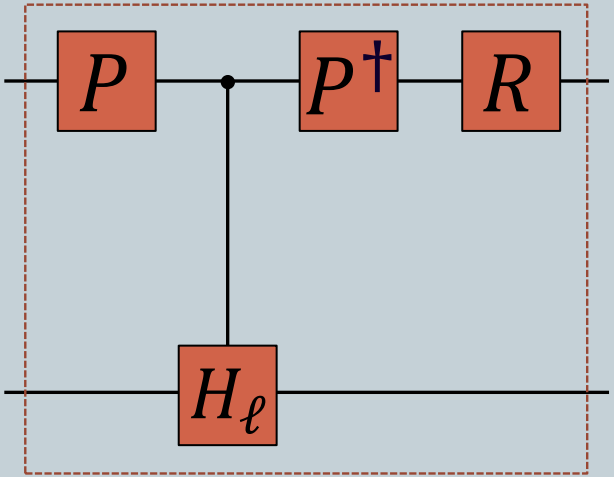

$$\lambda = \sum_{\ell} |w_\ell|$$

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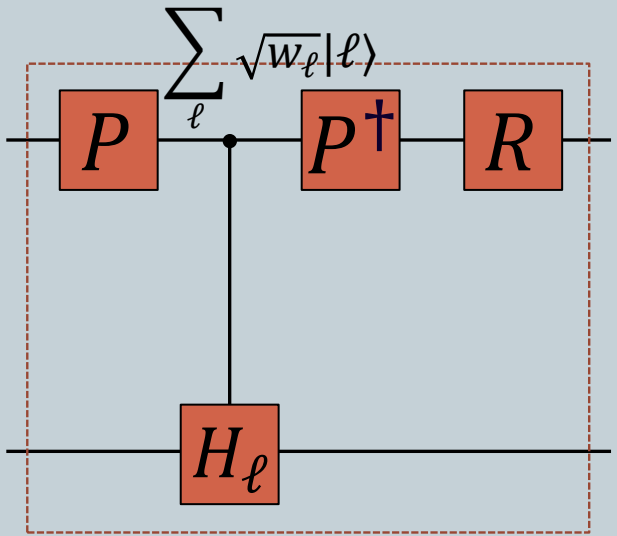

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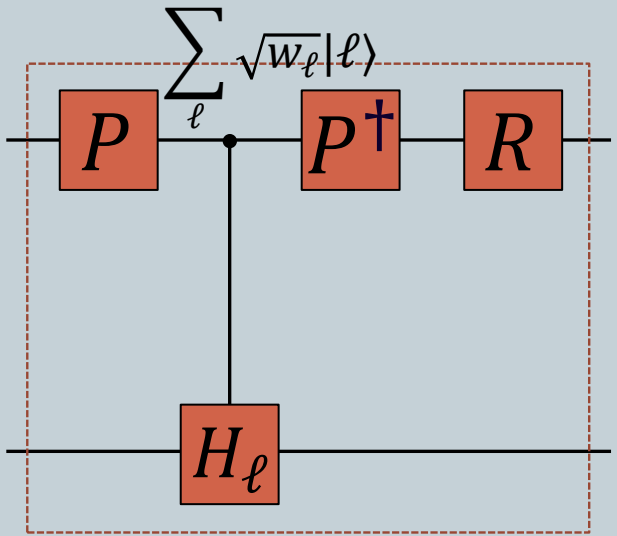
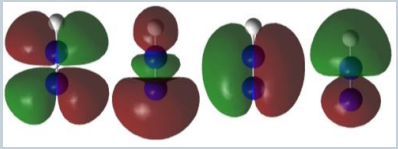


$$W \equiv e^{i \arcsin(H/\lambda)}$$

$$\lambda = \sum_{\ell} |w_\ell|$$

The electronic structure Hamiltonian



- To represent wavefunctions on computer we choose N orbitals.
- There are $O(N^4)$ Hamiltonian terms.

$$H = \sum_{p,q,r,s=1}^{N} V_{pqrs} a_p^\dagger a_q a_r^\dagger a_s + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

- $a_i^\dagger$ and a_j are creation and annihilation operators for electrons (fermions).

- Overall complexity goes like

$$\lambda \times \sqrt{\text{data in } H}$$

Single factorisation

- Rewrite as

$$H = \sum_{p,q,r,s=1}^{N} V_{pqrs} a_p^\dagger a_q a_r^\dagger a_s + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

$$= \sum_{\ell=1}^{L} \omega_\ell \left(\sum_{p,q=1}^{N} g_{pq}^{(\ell)} a_p^\dagger a_q \right)^2 + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

- Typically can take $L = O(N)$ – low rank.
- There are $O(N^3)$ parameters.

D. W. Berry, C. Gidney, M. Motta, J. McClean, R. Babbush, Quantum **3**, 208 (2019).

Double factorisation

- Rotate basis for each part of the factorisation:

$$\sum_{\ell=0}^{L} \omega_\ell \left(\sum_{p,q=1}^{N} g_{pq}^{(\ell)} a_p^\dagger a_q \right)^2 + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

$$\sum_{\ell=0}^{L} \omega_\ell U_\ell^\dagger \left(\sum_{m=1}^{M_\ell} h_{\ell m} n_m \right)^2 U_\ell + \sum_{\ell=1}^{N} t_\ell n_{\ell,T}$$

$$\sum_{\ell=0}^{L} \omega_\ell \left(\sum_{m=1}^{M_\ell} U_{\ell m}^\dagger h_{\ell m} n_1 U_{\ell m} \right)^2 + \sum_{\ell=1}^{N} t_\ell U_{\ell,T}^\dagger n_1 U_{\ell,T}$$

V. von Burg, G. H. Low, T. Häner, D. S. Steiger, M. Reiher, M. Roetteler, M. Troyer, arXiv:2007.14460 (2020).

Tensor hypercontraction (THC)

- Hamiltonian is

$$H = \frac{1}{2}\sum_{p,q,r,s=1}^{N} V_{pqrs} a_p^\dagger a_q a_r^\dagger a_s + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

$$\approx \frac{1}{2}\sum_{p,q,r,s=1}^{N}\sum_{\mu,\nu=1}^{M} \chi_p^{(\mu)} \chi_q^{(\mu)} \zeta_{\mu\nu} \chi_r^{(\nu)} \chi_s^{(\nu)} a_p^\dagger a_q a_r^\dagger a_s + \sum_{p,q=1}^{N} T_{pq} a_p^\dagger a_q$$

- Typically can take $M = O(N) \quad \Rightarrow$ number of parameters is $O(N^2)$.

- Number of steps would scale as

$$\lambda \propto \sum_{p,q,r,s=1}^{N}\sum_{\mu,\nu=1}^{M} \left| \chi_p^{(\mu)} \chi_q^{(\mu)} \zeta_{\mu\nu} \chi_r^{(\nu)} \chi_s^{(\nu)} \right|$$

E. G. Hohenstein, R. M. Parrish, T. J. Martínez, J. Chem. Phys. **137**, 044103 (2012).

Nonorthogonal basis

- For the two-electron part:

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\left(\sum_{p=1}^{N}\chi_p^{(\mu)}a_p^\dagger\right)\left(\sum_{q=1}^{N}\chi_q^{(\mu)}a_q\right)\zeta_{\mu\nu}\left(\sum_{r=1}^{N}\chi_r^{(\nu)}a_r^\dagger\right)\left(\sum_{s=1}^{N}\chi_s^{(\nu)}a_s\right)$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}c_\mu^\dagger c_\mu\zeta_{\mu\nu}c_\nu^\dagger c_\nu$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\zeta_{\mu\nu}n_\mu n_\nu$$

$$c_\mu=\sum_{q=1}^{N}\chi_q^{(\mu)}a_q$$

Nonorthogonal basis

- For the two-electron part:

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\left(\sum_{p=1}^{N}\chi_p^{(\mu)}a_p^\dagger\right)\left(\sum_{q=1}^{N}\chi_q^{(\mu)}a_q\right)\zeta_{\mu\nu}\left(\sum_{r=1}^{N}\chi_r^{(\nu)}a_r^\dagger\right)\left(\sum_{s=1}^{N}\chi_s^{(\nu)}a_s\right)$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}c_\mu^\dagger c_\mu\zeta_{\mu\nu}c_\nu^\dagger c_\nu$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\zeta_{\mu\nu}n_\mu n_\nu$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\zeta_{\mu\nu}\left(U_\mu^\dagger n_1 U_\mu\right)\left(U_\nu^\dagger n_1 U_\nu\right)$$

Nonorthogonal basis

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$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\left(\sum_{p=1}^{N}\chi_p^{(\mu)}a_p^\dagger\right)\left(\sum_{q=1}^{N}\chi_q^{(\mu)}a_q\right)\zeta_{\mu\nu}\left(\sum_{r=1}^{N}\chi_r^{(\nu)}a_r^\dagger\right)\left(\sum_{s=1}^{N}\chi_s^{(\nu)}a_s\right)$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}c_\mu^\dagger c_\mu\zeta_{\mu\nu}c_\nu^\dagger c_\nu$$

$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\zeta_{\mu\nu}n_\mu n_\nu$$

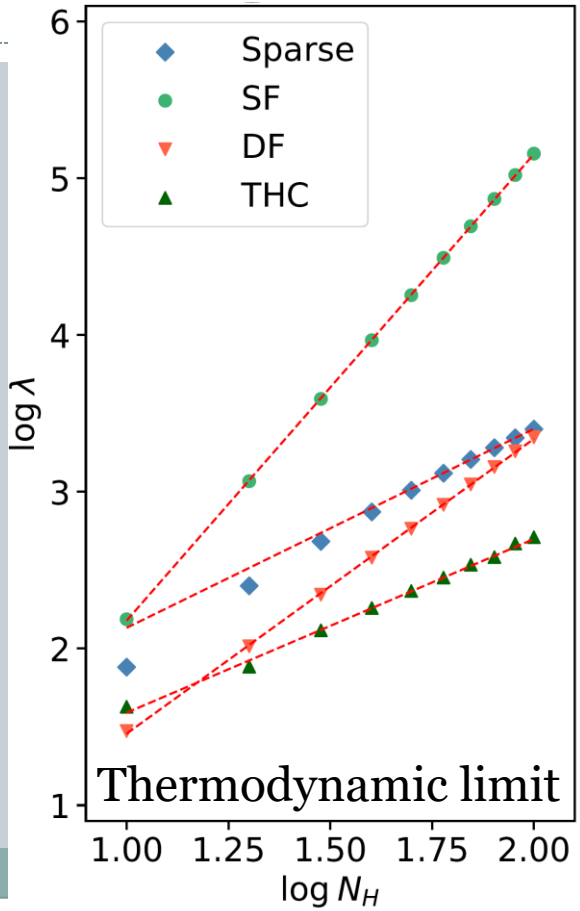
$$\frac{1}{2}\sum_{\mu,\nu=1}^{M}\zeta_{\mu\nu}\left(U_\mu^\dagger n_1 U_\mu\right)\left(U_\nu^\dagger n_1 U_\nu\right)$$

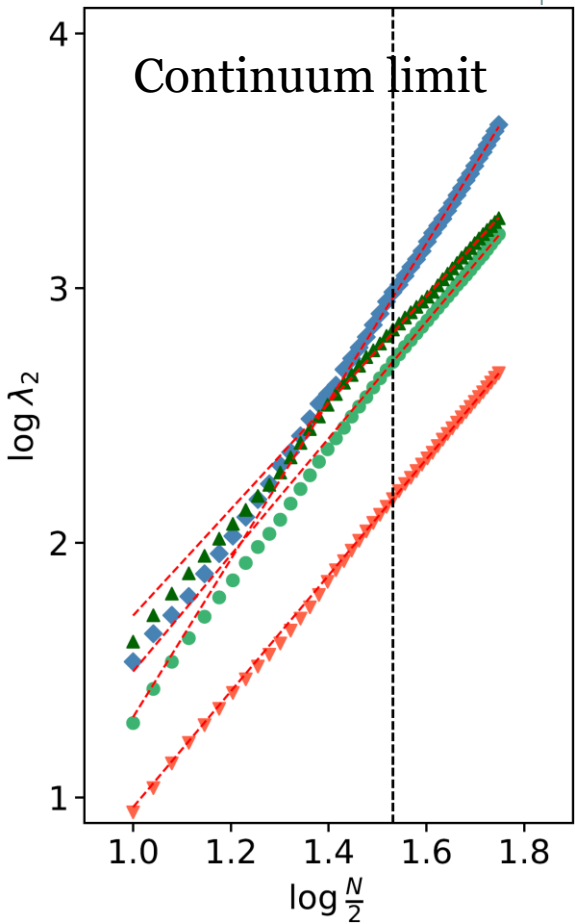
$$\lambda \propto \sum_{p,q,r,s=1}^{N}\sum_{\mu,\nu=1}^{M}\left|\chi_p^{(\mu)}\chi_q^{(\mu)}\zeta_{\mu\nu}\chi_r^{(\nu)}\chi_s^{(\nu)}\right|$$

$$\lambda \propto \sum_{\mu,\nu=1}^{M}\left|\zeta_{\mu\nu}\right|$$

Asymptotic λ

- Thermodynamic limit (growing system size)
  $N^{1.11}$ THC
  $N^{1.88}$ for DF
- Continuum limit (increasing orbitals for single system)
  $N^{2.09}$ THC
  $N^{2.28}$ for DF

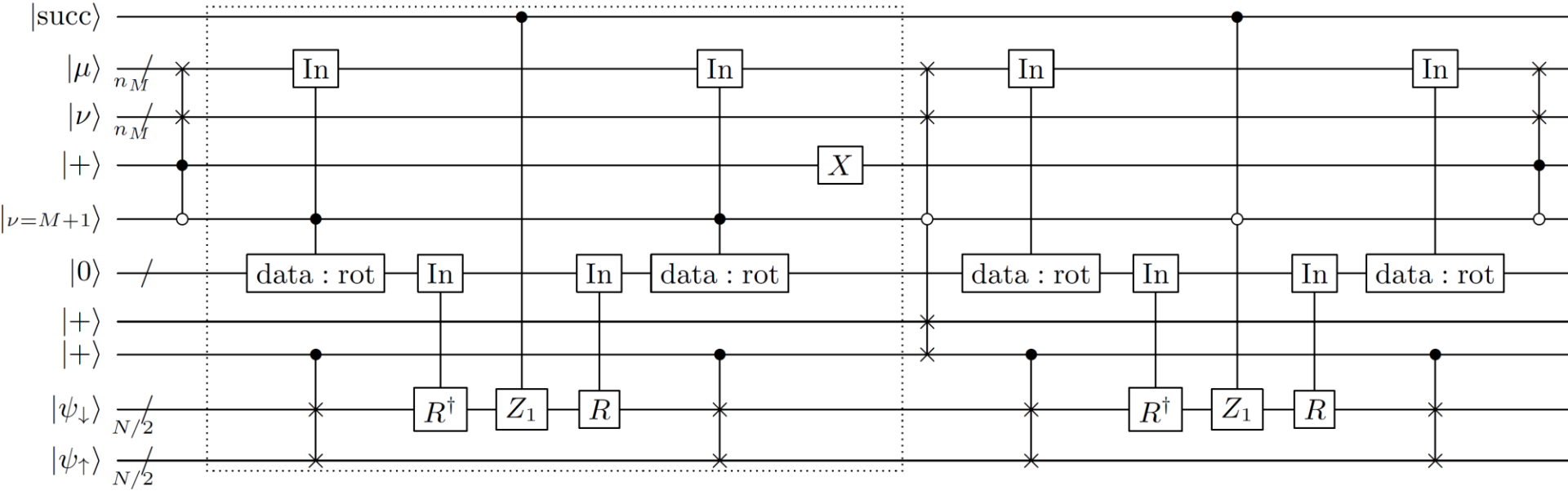




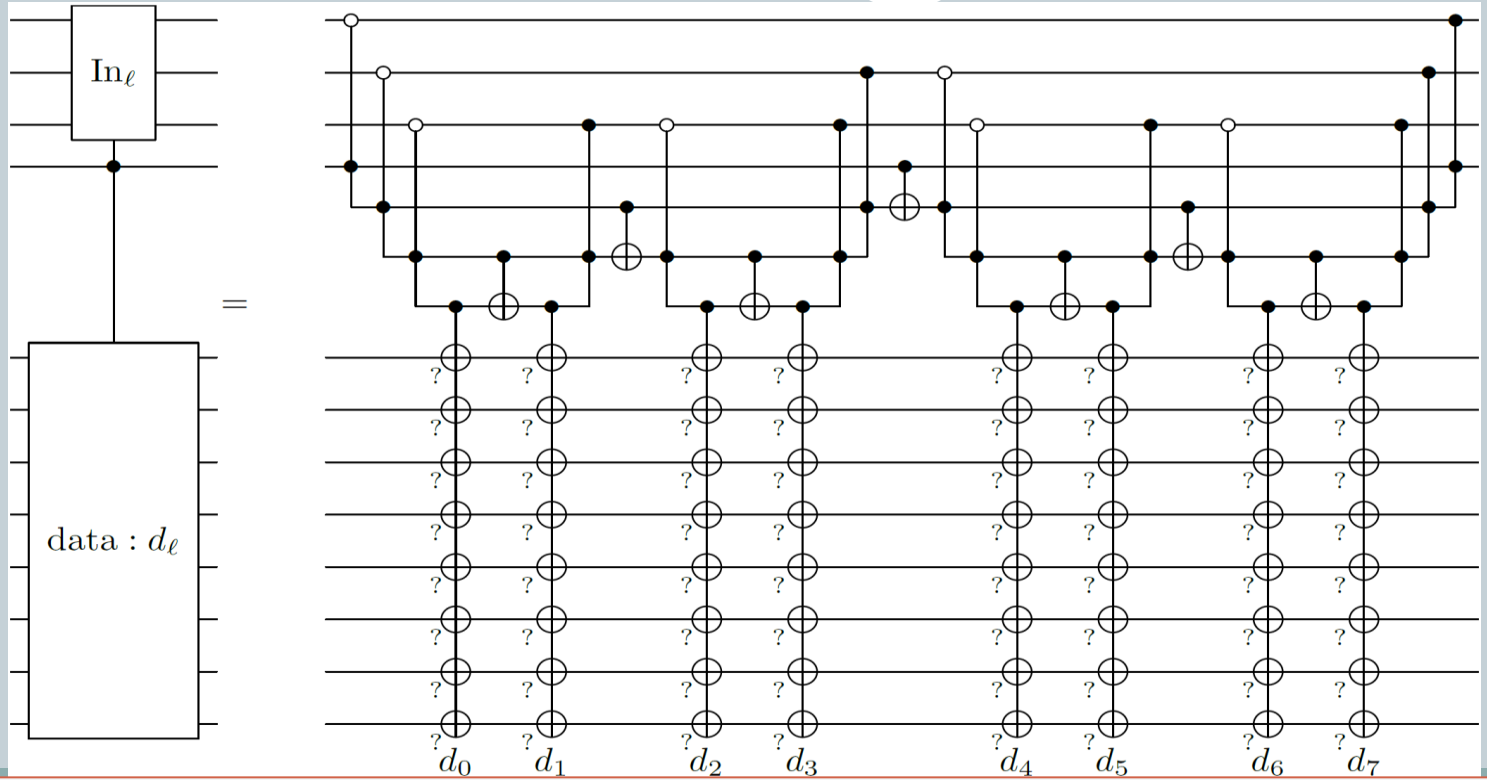
Majorana operators

- Each qubit records the occupation of an orbital, e.g.
  $|\psi\rangle = \alpha_1|0011\rangle + \alpha_2|0101\rangle + \alpha_3|1001\rangle + \alpha_4|0110\rangle + \alpha_5|1010\rangle + \alpha_6|1100\rangle$
- Anticommuting Majorana operators:
  $$\gamma_{p0} = a_p + a_p^\dagger \qquad \gamma_{p1} = -i(a_p - a_p^\dagger)$$
- Use the Jordan-Wigner transformation:
  $$\gamma_{p0} = X_p Z_{p-1} Z_{p-2} \cdots Z_0 \qquad \gamma_{p1} = Y_p Z_{p-1} Z_{p-2} \cdots Z_0$$
  $$n_p = (\mathbb{I} - Z_p)/2$$
- Two-body part of Hamiltonian becomes
  $$\frac{1}{8} \sum_{\mu,\nu=1}^{M} \zeta_{\mu\nu} \left(U_\mu^\dagger Z_1 U_\mu\right)\left(U_\nu^\dagger Z_1 U_\nu\right)$$

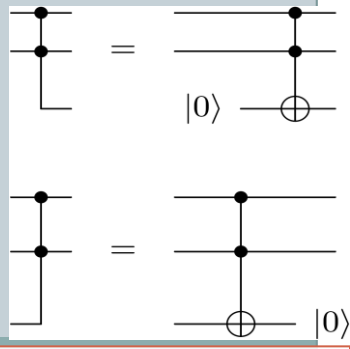
The controlled unitary



Quantum ROM



Gidney's joint trick



R. Babbush, C. Gidney, D. W. Berry, N. Wiebe, J. McClean, A. Paler, A. Fowler, H. Neven, Physical Review X **8**, 041015 (2018).

Coherent alias sampling

- We aim to prepare

$$\sum_{\ell=1}^{L} \sqrt{\frac{w_\ell}{\lambda}} |\ell\rangle$$

- We can allow entanglement with an ancilla

$$\sum_{\ell=1}^{L} \sqrt{\frac{w_\ell}{\lambda}} |\ell\rangle |\mathrm{temp}_\ell\rangle$$

- For each ℓ we determine an alternate value alt_ℓ and a probability keep_ℓ.

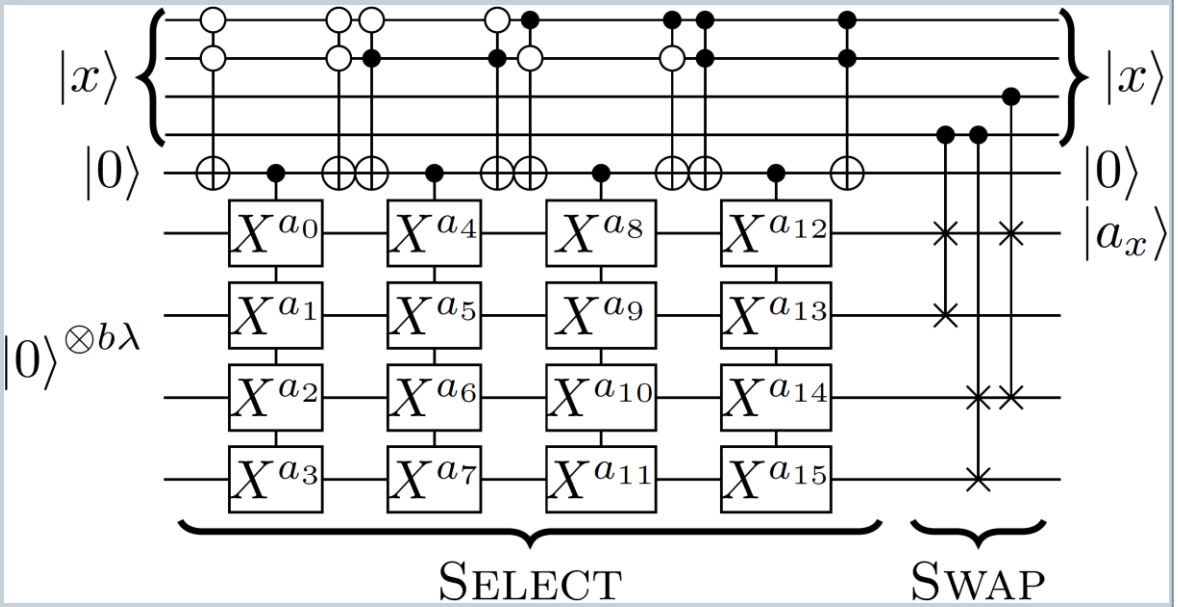
$$\sum_{\ell=1}^{L} \sqrt{\frac{1}{L}} |\ell\rangle |\mathrm{alt}_\ell\rangle |\mathrm{keep}_\ell\rangle$$

- We swap register $|\ell\rangle$ with register $|\mathrm{alt}_\ell\rangle$ with probability $|\mathrm{keep}_\ell\rangle$.

R. Babbush, C. Gidney, D. W. Berry, N. Wiebe, J. McClean, A. Paler, A. Fowler, H. Neven, Physical Review X **8**, 041015 (2018).

Advanced QROM

- Regular QROM would use L Toffolis for L data points.
- Instead use two step process:
  1. Iterate through bits ignoring lowest $\log k$ bits; complexity L/k.
  2. Swap data based on remaining $\log k$ bits; complexity $m(k-1)$ for size-m output.
- Optimal $k \sim \sqrt{L/m}$ gives complexity $O(\sqrt{Lm})$.
- $O(\sqrt{Lm})$ ancillas needed.

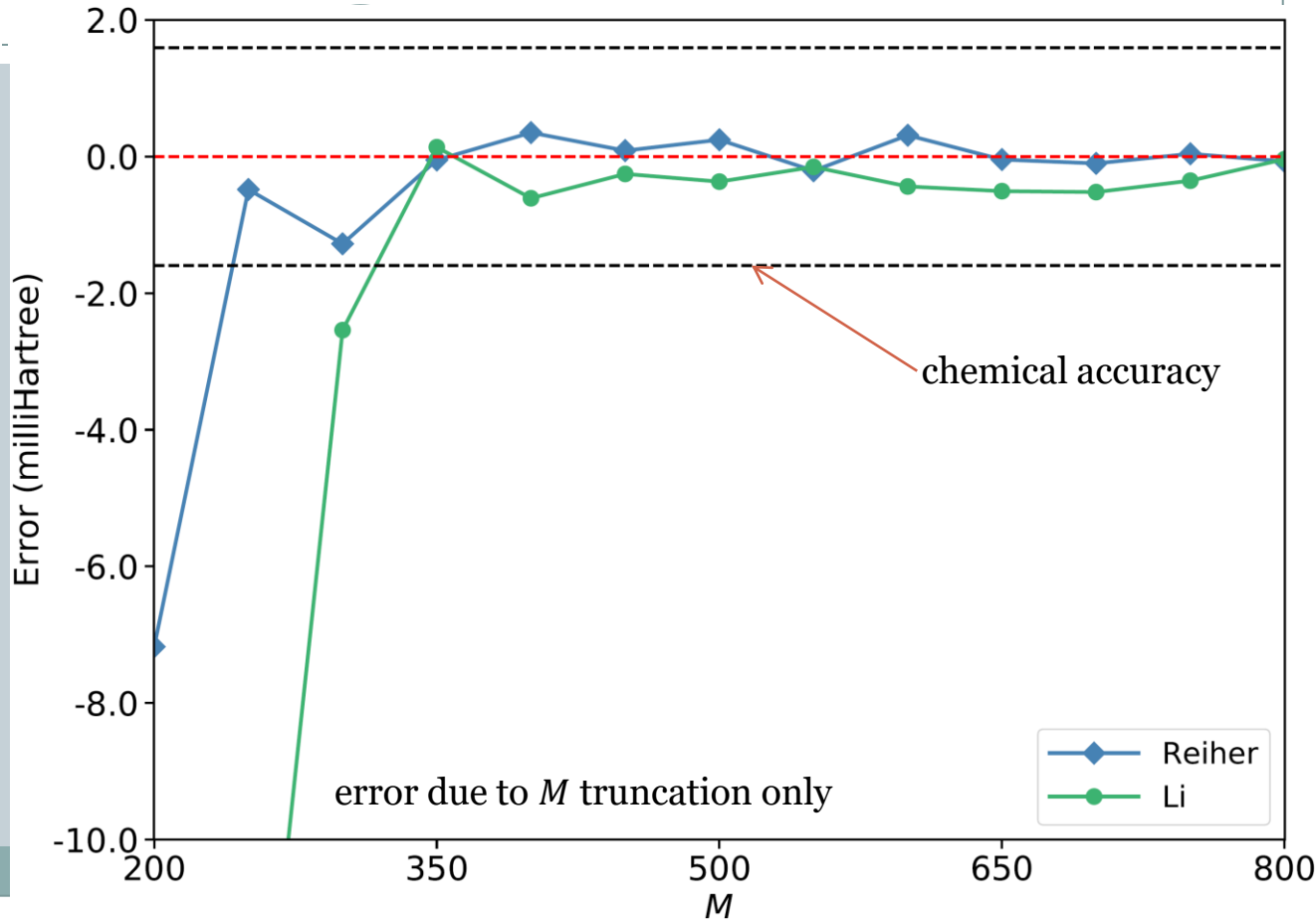


G. H. Low, V. Kliuchnikov, L. Schaeffer, arXiv:1812.00954 (2018).

Approximating the Hamiltonian

Two types of orbitals:

- Reiher *et al.* [PNAS **114**, 7555 (2017)]
  $N = 108$
- Li *et al.* [J Chem Phys **150**, 024302 (2019)]
  $N = 152$



Resulting complexities (FeMoco)

Total error 1.6 mHa: 1 mHa for phase estimation + 0.6 mHa for approximation of the Hamiltonian

Reiher:

- $M = 350$
- 16 bits for rotations
- 10 bits for state preparation
- Hamiltonian error 0.29 mHa
- $\lambda = 306.3$
- 2142 logical qubits
- 5.3 billion Toffolis

Li:

- $M = 450$
- 20 bits for rotations
- 10 bits for state preparation
- Hamiltonian error 0.18 mHa
- $\lambda = 1201.5$
- 2196 logical qubits
- 32 billion Toffolis

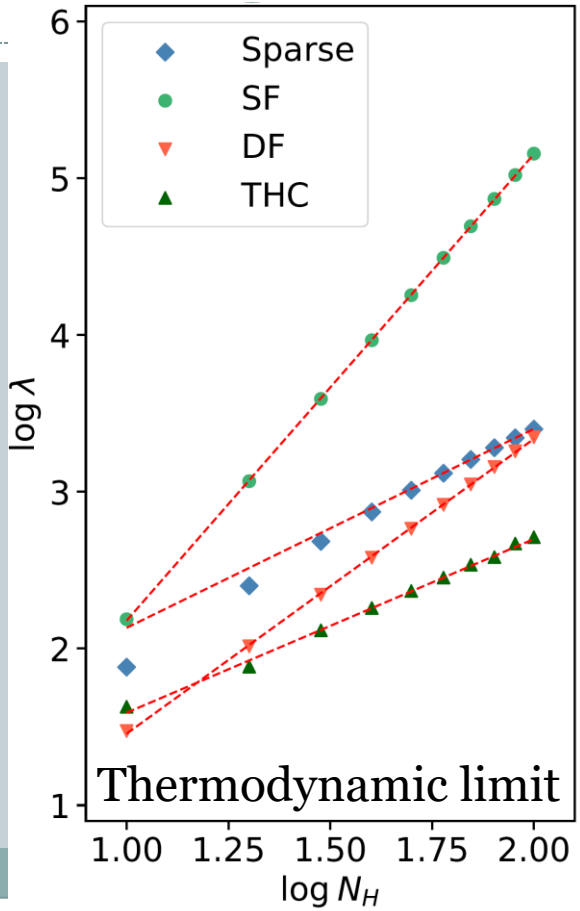
Comparison to other methods (FeMoco)

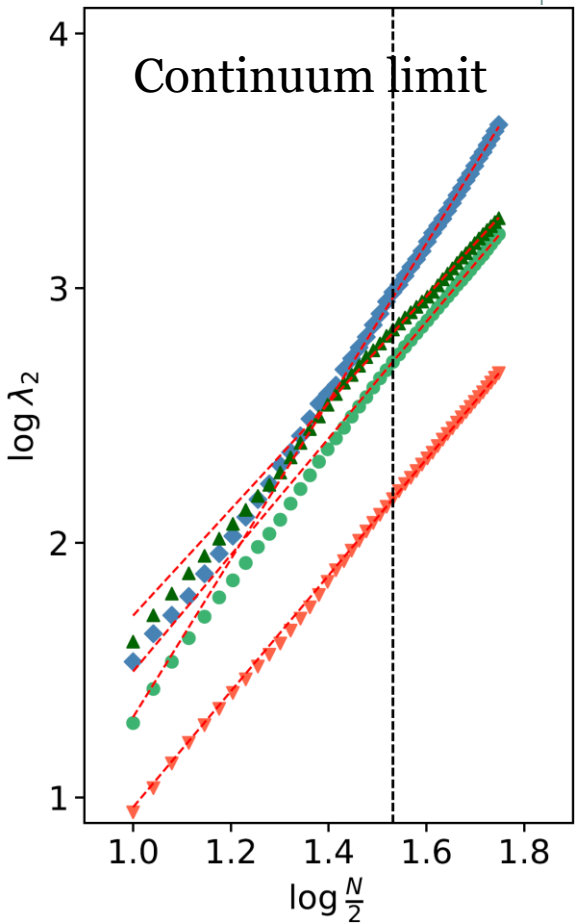
- For prior methods we allowed the same precision for a fair comparison.
- We corrected and improved state preparation for double factorisation.
- We corrected λ for our sparse method, and further optimised it.
- We improved our single factorisation method with amplitude amplification.

Algorithm	Reiher		Li	
	qubits	Toffolis (billions)	qubits	Toffolis (billions)
single factorisation	3320	95	3628	120
sparse	2190	88	2489	44
double factorisation (von Burg)	3725	10	6404	64
tensor hypercontraction	2142	5.3	2196	32

Asymptotics

- Complexity $\lambda \times \sqrt{\text{data}}$
- THC data $\tilde{O}(N^2)$
- DF data $\tilde{O}(N^3)$
- Thermodynamic limit
  THC: $N^{1.11} \times \sqrt{N^2} \sim N^{2.1}$
  DF: $N^{1.88} \times \sqrt{N^3} \sim N^{3.4}$
- Continuum limit
  THC: $N^{2.1} \times \sqrt{N^2} \sim N^{3.1}$
  DF: $N^{2.3} \times \sqrt{N^3} \sim N^{3.8}$





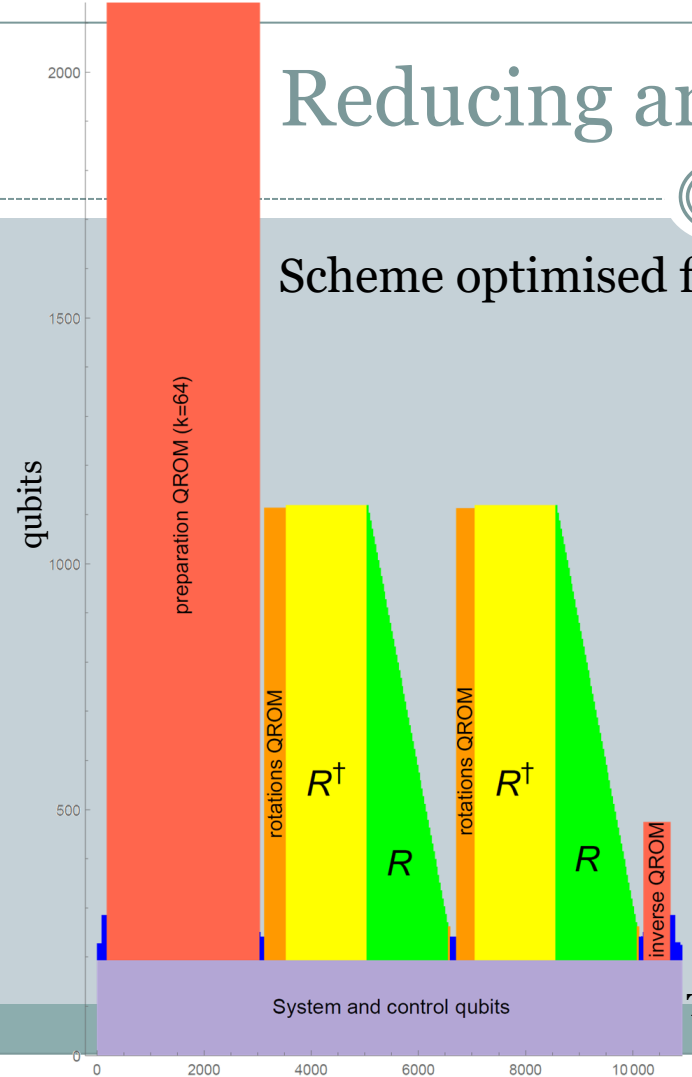
Progression of complexities

Algorithm	H chain thermodynamic limit (as system grows)	H_4 continuum limit (increasing precision)
Taylor series database [1]	$\tilde{O}(N^{5.3}/\epsilon)$	$\tilde{O}(N^{7.1}/\epsilon)$
Campbell qDRIFT [2,3]	$\tilde{O}(N^{2.5}/\epsilon^2)$	$\tilde{O}(N^{6.2}/\epsilon^2)$
Single factorisation [4]	$\tilde{O}(N^{4.5}/\epsilon)$	$\tilde{O}(N^{3.8}/\epsilon)$
Sparse [4]	$\tilde{O}(N^{2.3}/\epsilon)$	$\tilde{O}(N^{5.0}/\epsilon)$
Double factorisation [5]	$\tilde{O}(N^{3.4}/\epsilon)$	$\tilde{O}(N^{3.8}/\epsilon)$
THC (this work) [6]	$\tilde{O}(N^{2.1}/\epsilon)$	$\tilde{O}(N^{3.1}/\epsilon)$

[1] R. Babbush, D. W. Berry, I. D. Kivlichan, A. Y. Wei, P. J. Love, A. Aspuru-Guzik, New Journal of Physics **18**, 33032 (2016).
[2] E. Campbell, Physical Review Letters **123**, 070503 (2019).
[3] I. D. Kivlichan, C. E. Granade, N. Wiebe, arXiv:1907.10070 (2019).
[4] D. W. Berry, C. Gidney, M. Motta, J. McClean, R. Babbush, Quantum **3**, 208 (2019).
[5] V. von Burg, G. H. Low, T. Häner, D. S. Steiger, M. Reiher, M. Roetteler, M. Troyer, arXiv:2007.14460 (2020).
[6] J. Lee, D. W. Berry, C. Gidney, W. J. Huggins, J. R. McClean, N. Wiebe, R. Babbush, arXiv: 2011.03494 (2020).

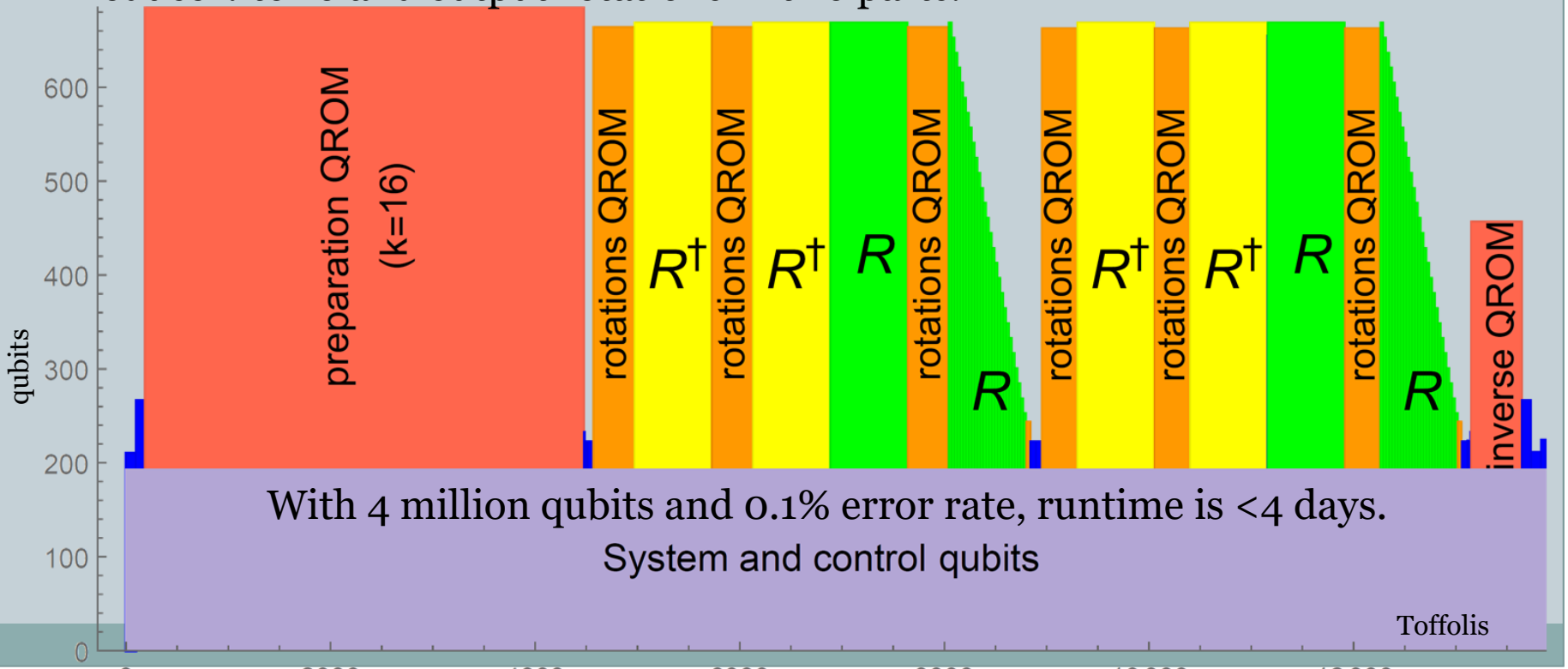
Reducing ancillas needed

Scheme optimised for Toffolis.



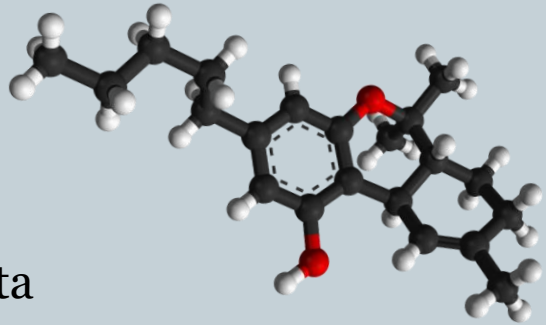
Reducing ancillas needed

Reduce k to 16 and output rotations in two parts.



Conclusions

- We get the highest efficiency yet with THC (tensor hypercontraction).
- The efficiency is high because:
  1. Hamiltonian λ-norm is small
  2. Hamiltonian is represented with a small amount of data
- Projected scaling for larger systems $N^{2.1}$ is the best yet.
- For FeMoco the complexity is down to 5 billion Toffolis.



J. Lee, D.W. Berry, C. Gidney, W.J. Huggins, J.R. McClean, N. Wiebe, R. Babbush, arXiv: 2011.03494 (2020).