



A quantum computing perspective on many-body methods

Nicholas Rubin

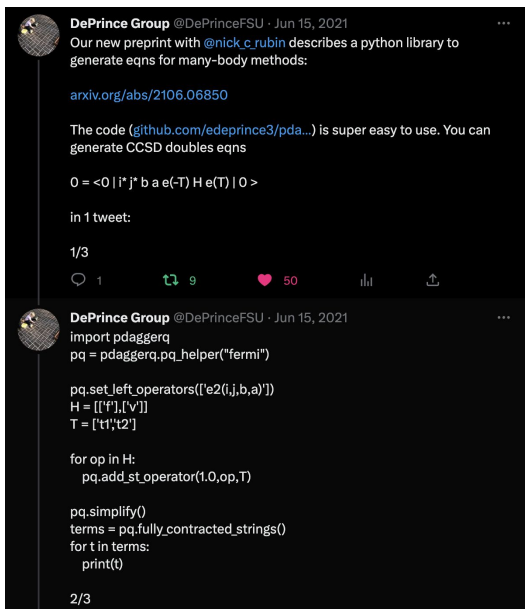
ENST “Workshop Automated tools for many-body theory”

June 7, 2023



$p^{\dagger}q$: A tool for prototyping many-body methods for quantum chemistry

- automated equation and code generation for many-body quantum chemistry methods
- support for :
 - normal order with respect to the true vacuum or the fermi vacuum
 - CC-type objects (T, L, R) with up to four-body transitions
 - EE- / EA- / IP-type EOM-CC objects
 - Python einsum implementations (current) and C++ TiledArray implementations (coming soon)
 - Cavity QED EOM-CC



DePrince Group @DePrinceFSU · Jun 15, 2021

Our new preprint with @nick_c_rubin describes a python library to generate eqns for many-body methods:

arxiv.org/abs/2106.06850

The code (github.com/edeprince3/pda...) is super easy to use. You can generate CCSD doubles eqns

$$O = \langle 0 | i^* j^* b a e(-T) H e(T) | 0 \rangle$$

in 1 tweet:

1/3

1 9 50

DePrince Group @DePrinceFSU · Jun 15, 2021

```
import pdaggerq
pq = pdaggerq.pq_helper("fermi")

pq.set_left_operators(["e2(i,j,b,a)"])
H = [{"f"}, {"v"}]
T = ["t1", "t2"]

for op in H:
    pq.add_st_operator(1.0, op, T)

pq.simplify()
terms = pq.fully_contracted_strings()
for t in terms:
    print(t)
```

2/3



<https://github.com/edeprince3/pdaggerq>

N. C. Rubin and A. E. DePrince III, *Mol. Phys.* **119**, e1954709 (2021)

$p^{\dagger}q$: A tool for prototyping many-body methods for quantum chemistry

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```
# import pdaggerq
import pdaggerq

# import equation parser
from pdaggerq.parser import contracted_strings_to_tensor_terms

# grab pq_helper for fermio vacuum
pq = pdaggerq.pq_helper("fermi")

# ccSD doubles residual

# set bra
pq.set_left_operators([[e2(i,j,b,a)]]])

# add similarity-transform hamiltonian
pq.add_st_operator(1.0,['f'],['t1', 't2'])
pq.add_st_operator(1.0,['v'],['t1', 't2'])

pq.simplify()

# grab list of fully-contracted strings, then print
terms = pq.fully_contracted_strings()
for my_term in terms:
    print(my_term)

# python code
terms = contracted_strings_to_tensor_terms(terms)
for my_term in terms:
    print("#t", my_term)
    print("%s" % (my_term.einsum_string(update_val='doubles_res',
                                     output_variables=('a', 'b', 'i', 'j'))))
    print()

pq.clear()
```

```
(16:36 ~/) python ccSD.py
[-1.0000000000000000, 'P(i,j)', 'f(k,j)', 't2(a,b,i,k)']
[+1.0000000000000000, 'P(a,b)', 'f(a,c)', 't2(c,b,i,j)']
[-1.0000000000000000, 'P(i,j)', 'f(k,c)', 't1(c,j)', 't2(a,b,i,k)']
[-1.0000000000000000, 'P(a,b)', 'f(k,c)', 't1(a,k)', 't2(c,b,i,j)']
[+1.0000000000000000, '<a,b||i,j>']

...

#
-1.0000 P(i,j)f(k,c)*t2(a,b,i,k)
contracted_intermediate = -1.0000000000000000 * einsum('kj,abik->abij', f[o, o], t2)
doubles_res += 1.00000 * contracted_intermediate + -1.00000 * einsum('abij->abji', contracted_intermediate)

#
1.0000 P(a,b)f(a,c)*t2(c,b,i,j)
contracted_intermediate = 1.0000000000000000 * einsum('ac,cbij->abij', f[v, v], t2)
doubles_res += 1.00000 * contracted_intermediate + -1.00000 * einsum('abij->baij', contracted_intermediate)

#
-1.0000 P(i,j)f(k,c)*t1(c,j)*t2(a,b,i,k)
contracted_intermediate = -1.0000000000000000 * einsum('kc,cj,abik->abij', f[o, v], t1, t2, optimize='einsum_path', (0, 1), (0, 1))
doubles_res += 1.00000 * contracted_intermediate + -1.00000 * einsum('abij->abji', contracted_intermediate)

#
-1.0000 P(a,b)f(k,c)*t1(a,k)*t2(c,b,i,j)
contracted_intermediate = -1.0000000000000000 * einsum('kc,ak,cbij->abij', f[o, v], t1, t2, optimize='einsum_path', (0, 1), (0, 1))
doubles_res += 1.00000 * contracted_intermediate + -1.00000 * einsum('abij->baij', contracted_intermediate)

#
1.0000 <a,b||i,j>
doubles_res += 1.0000000000000000 * einsum('abij->abij', g[v, v, o, o])

...
```



<https://github.com/edeprince3/pdaggerq>

N. C. Rubin and A. E. DePrince III, *Mol. Phys.* **119**, e1954709 (2021)

Qubits and gates, briefly

Any 2-state quantum system is a qubit, $|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle$

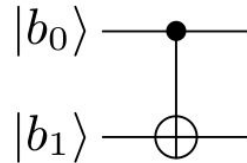
For 2 qubits, $|\psi\rangle = a_{00} |00\rangle + a_{01} |01\rangle + a_{10} |10\rangle + a_{11} |11\rangle$

N qubit systems requires $O(2^N)$ classical bits to represent

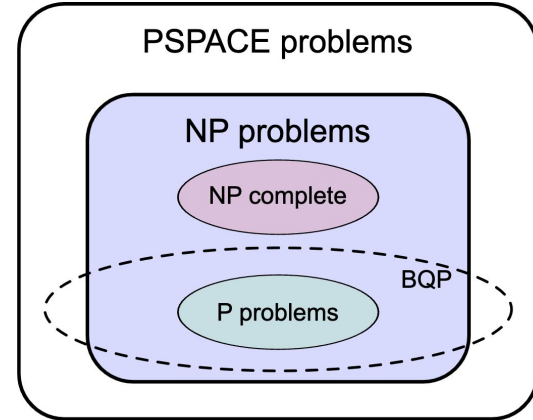
Information manipulated by controlled Hamiltonian evolutions

For instance, evolve 2 qubits under $H = (Z_0 - I_0) \otimes (I_1 - X_1)$ for time, $t = \pi/4$

$$e^{-iHt} : |b_0\rangle |b_1\rangle \mapsto |b_0\rangle |b_0 \oplus b_1\rangle$$

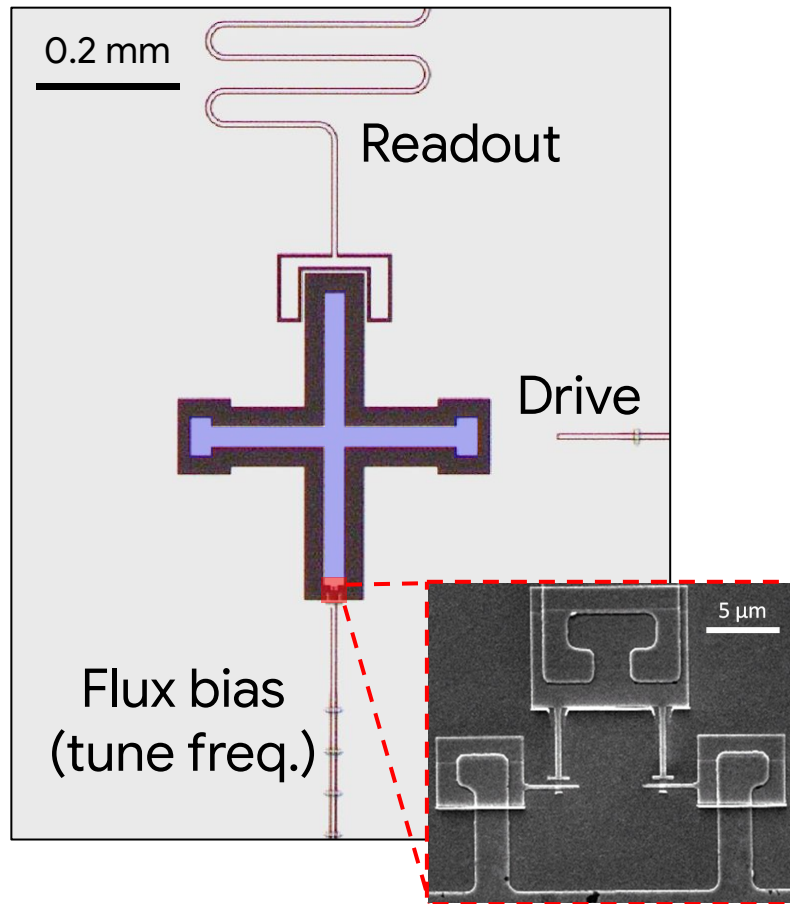
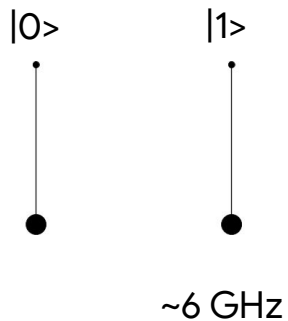
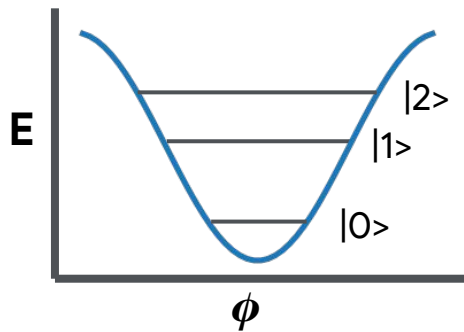
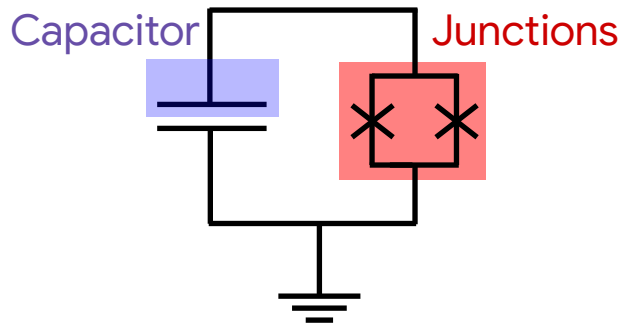


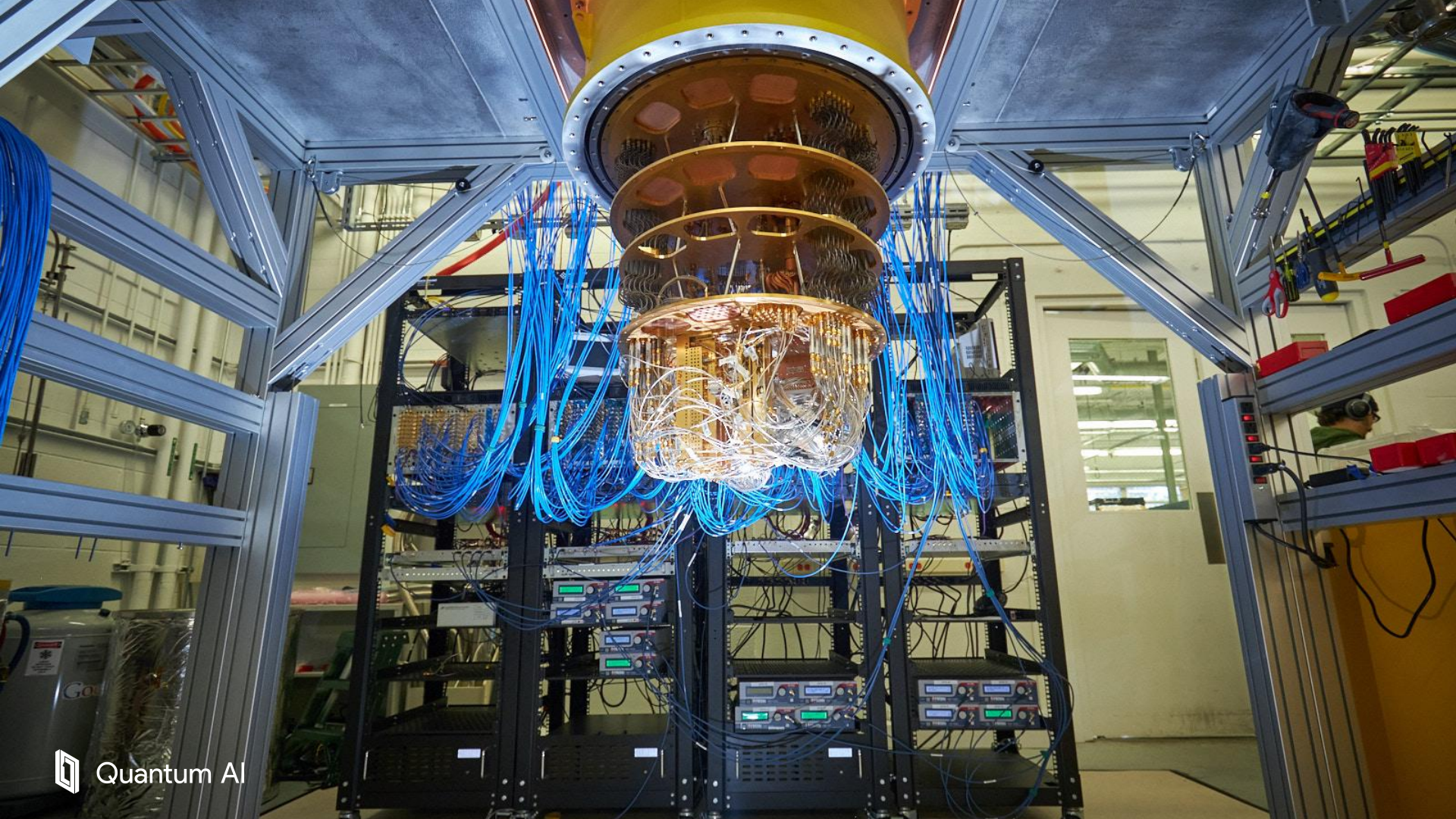
CNOT + single qubit rotations “universal” for all quantum dynamics / circuits



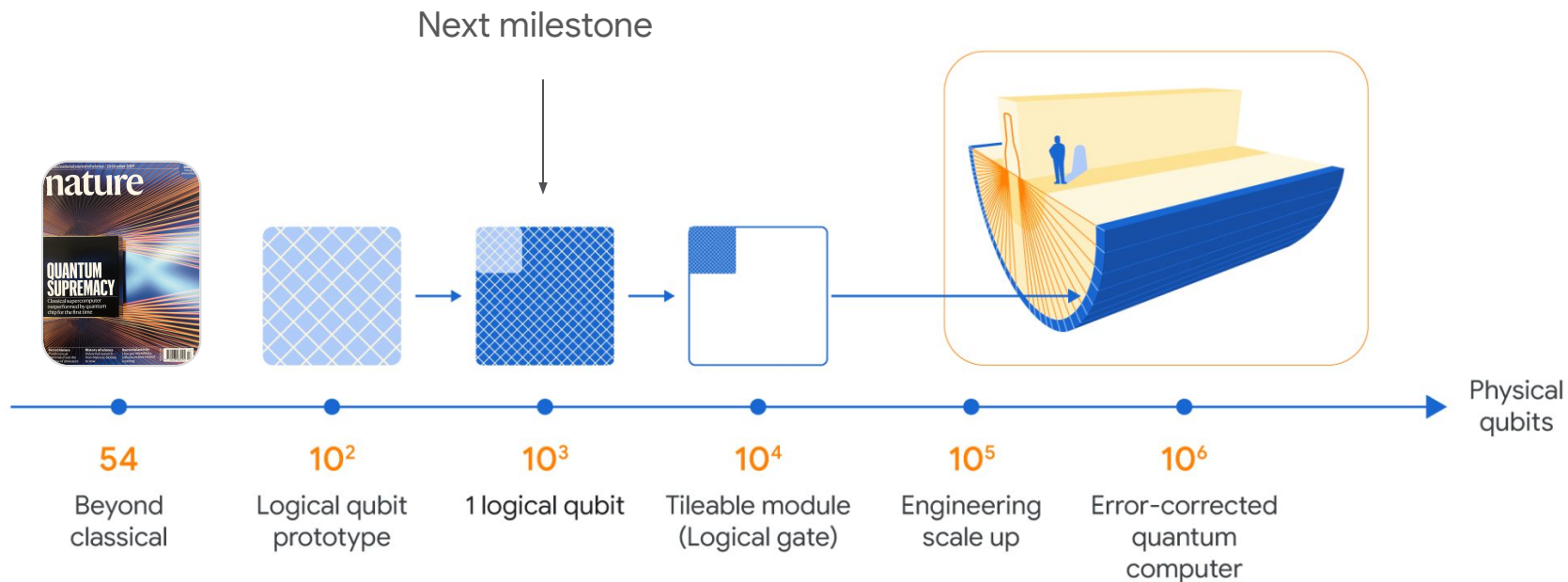
“Transmon” qubit

Nonlinear
superconducting
oscillator





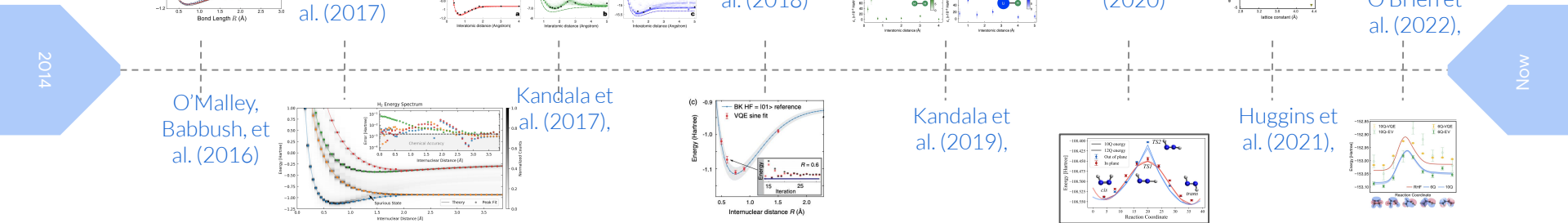
Google's roadmap to fault-tolerant quantum computing



Are we on a path to qchem simulation advantage?

We are in the age of noisy intermediate scale (NISQ) quantum devices

We can run circuits on ~50 qubits but errors severely limit circuit size

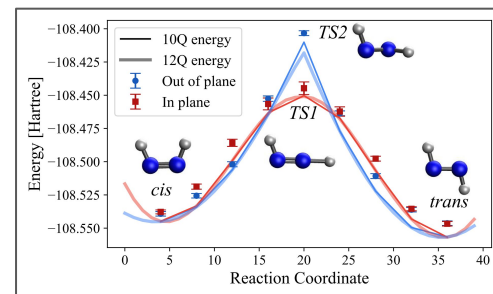
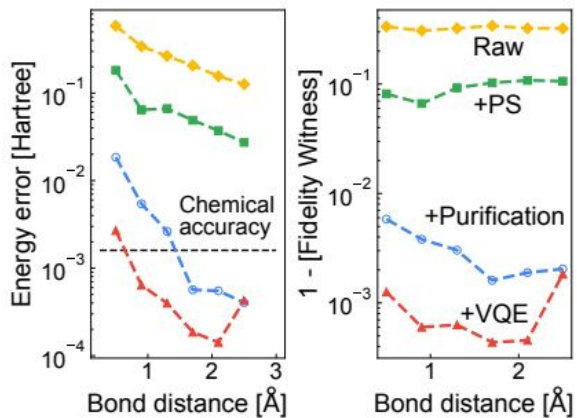
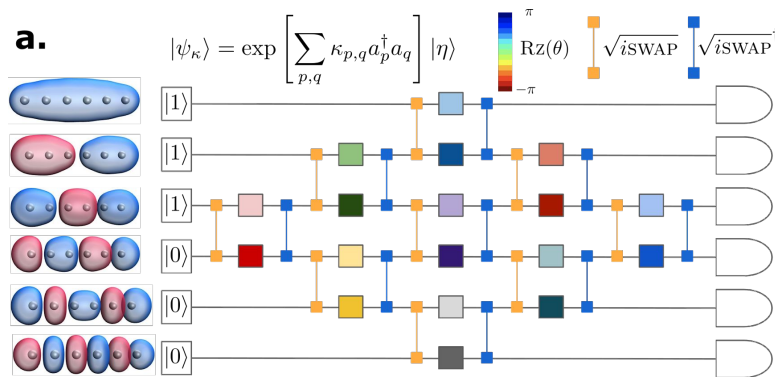


Experimental explorations are alive and well

Experiments are a playground for validating error mitigation and provable results

Hartree-Fock on a superconducting qubit quantum computer

- Largest variational quantum algorithm to date
- Primitive for quantum computing algorithms (Givens rotation)
- Non-interacting fermions:
 - Classically simulable :(
 - Free gradient estimation :)
 - McWeeny purification :)



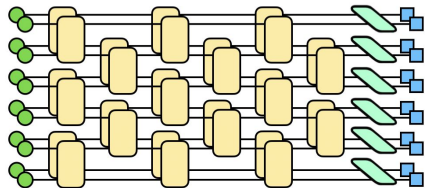
Rigorous results in NISQ

Error mitigation

Doubling in space: Virtual distillation

Phys. Rev. X 11, 041036 (2021)

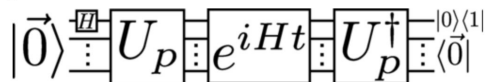
Circuit reps $\propto 1/f^4$



Doubling in time: Verified phase estimation

PRX Quantum 2, 020317 (2021)

Circuit reps $\propto 1/f^2$



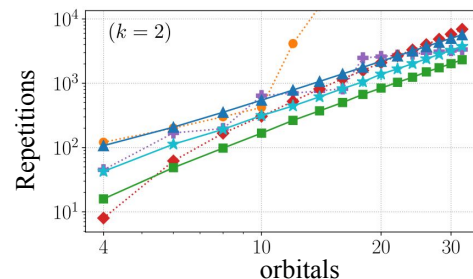
Measurement complexity

Optimal deterministic measurement complexity 1-RDM, 2-RDM, k-RDM

Science 369 1084-1089 (2021), Phys. Rev. X 10, 031064 (2020), Quantum, 4, 276.

SORTED INSERTION	n -qubit Clifford circuits $C \sim \mathcal{O}(n^{2k-1})$ (empirical)
Majorana clique cover	Ferm. Gaussian circuits $C = \mathcal{O}(n^k)$ ($k \leq 2$)
Fermionic swap networks	Basis-rotation circuits $C = \tilde{\mathcal{O}}(n^k)$
Classical shadows (FGU)	Ferm. Gaussian circuits $K_r/r = \tilde{\mathcal{O}}(n^k)$
Classical shadows (NC)	Basis-rotation circuits $K_r/r = \mathcal{O}(n^k)$

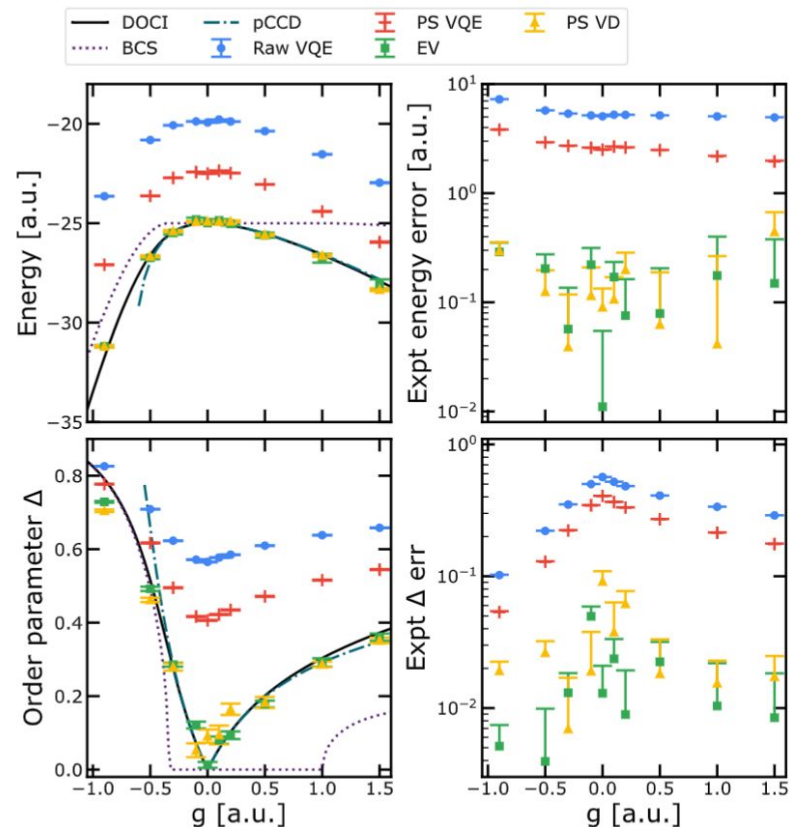
$$M = \mathcal{O} \left[\binom{n}{k} \frac{k^{3/2} \log n}{\epsilon^2} \right]$$



The Richardson-Gaudin model (10 sites)

$$H = \sum_{j,\alpha} j n_{j,\alpha} + g \sum_{j,k} c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{k\downarrow} c_{k\uparrow}$$

- Qualitatively accurate for Δ (superconducting order parameter)
- EV \sim PS-VD in performance.
- Mean improvement 50x over Raw VQE
- Error stable across range of g values, unlike classical methods (pccd, BCS).



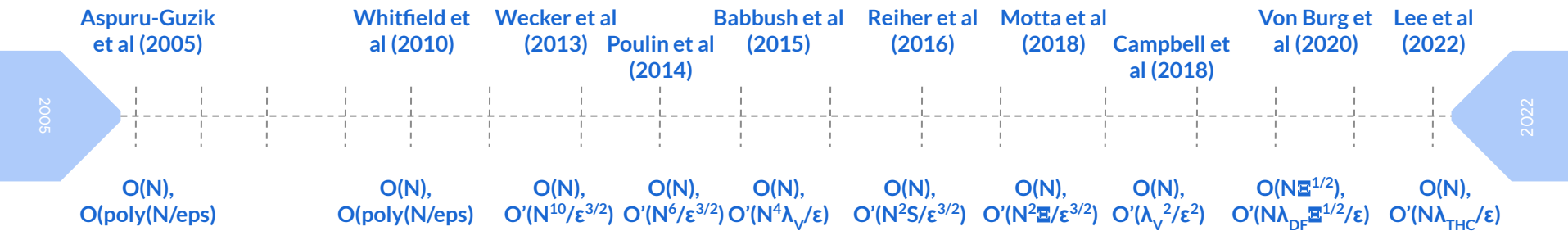
Summary of NISQ Progress

- VQE is very popular but progress in chemistry has been slow and the approach is very difficult to scale
- The number of measurements required quickly becomes problematically large
- Most compelling ansatz require circuits far too deep
- Theoretical basis for error mitigation can though needs to be verified in practice
- Different strategies (QC-QMC) are needed [Lee et al. Nature 603 (2022)]

Molecule	# Qubits	Year
H ₂	2	2014
H ₂ O	5	2020
BeH ₂	6	2017
N ₂ H ₂	10*	2020
H ₁₂	12*	2020



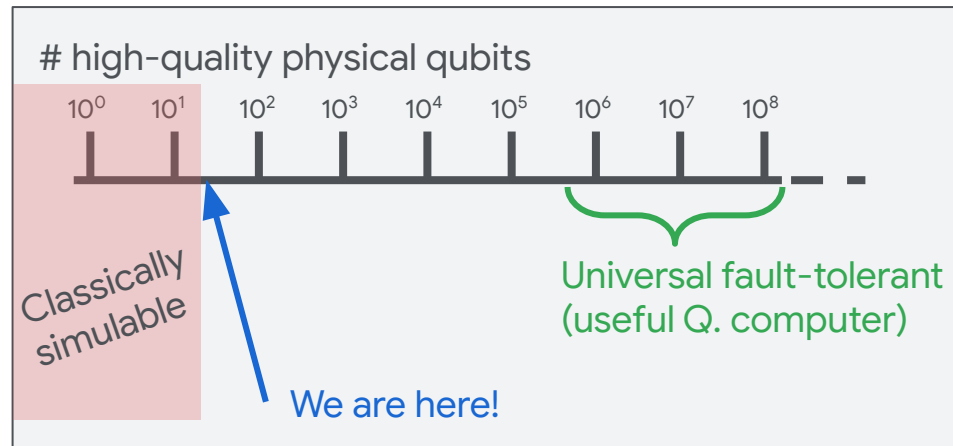
Are we on a path to qchem simulation advantage?



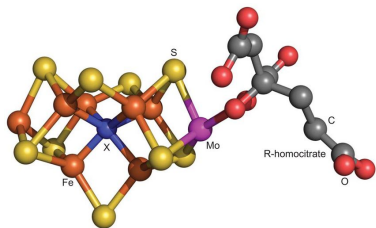
Theoretical progress in QPE going strong

Scaling in chemically relevant parameters are now close to optimal

Time for an honest assessment of progress?

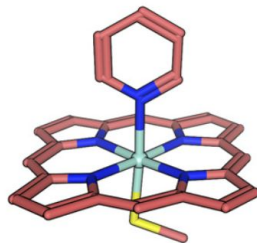


Quantum simulation advantage?



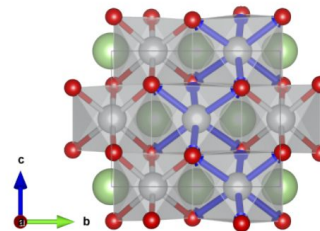
FeMoCo (fertilizer catalyst)
[PRX Quantum 2 \(3\), 030305](#)

4 M qubits
4 Days of runtime



P450 (drug anti-target)
[PNAS 119 \(38\), e2203533119](#)

4.6 M qubits
3 Days of runtime



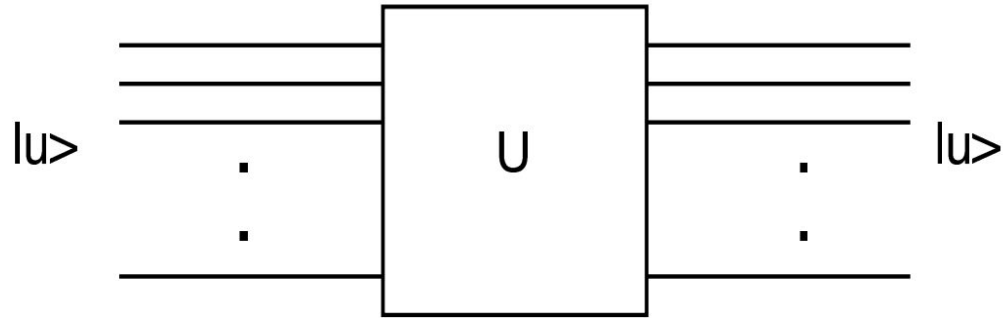
LiNiO₂ (battery cathode)
[arXiv:2302.05531](#)

? M qubits
? Days of runtime

Simulating Quantum Mechanics on a Quantum Computer

Phase Estimation Algorithm

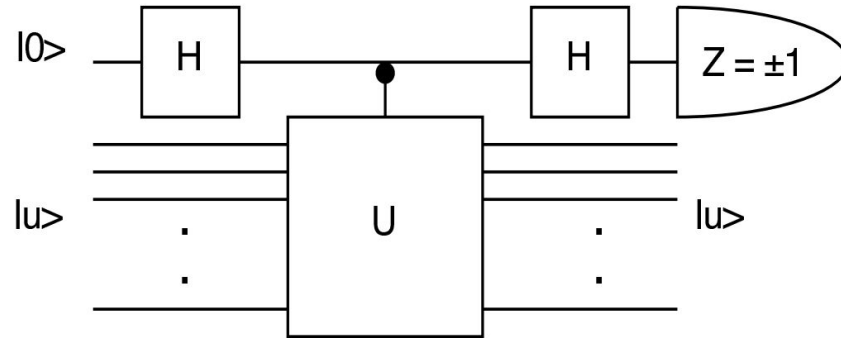
Time-evolution of eigenstate encodes the eigenvalues
in phase information



Simulating Quantum Mechanics on a Quantum Computer

Phase Estimation Algorithm

Time-evolution of eigenstate encodes the eigenvalues in phase information



$$\langle \hat{Z} \rangle = \langle u | (\hat{U} + \hat{U}^\dagger) | u \rangle / 2 = \frac{1}{2} (e^{2\pi i \phi} + e^{-2\pi i \phi}) = \cos(2\pi \phi)$$

Error-corrected quantum chemistry simulation

Science 309:5741 (2005), 1704-1707

1. Prepare an ansatz wavefunction ψ with “reasonable” support on the ground state

$$H |k\rangle = E_k |k\rangle \quad |\langle \psi | 0 \rangle|^2 = \text{not-too-small}$$

2. Form quantum circuit $U = e^{-if(H)}$ that encodes Hamiltonian spectrum in its eigenvalues

e.g., for Trotter:

$$f(H) = H = \sum_{\ell} H_{\ell} \quad U \approx \left(\prod_{\ell} e^{-iH_{\ell}/r} \right)^r$$

3. Application of U to ψ accumulates phases $f(E)$ encoding the spectrum

$$U |\psi\rangle = \sum_k \underbrace{\langle k | \psi \rangle}_{a_k} e^{-if(E_k)} |k\rangle$$

4. Phase estimation gives E_0 with error ϵ and probability $|a_0|^2$ using $\frac{1}{\epsilon} \left\| \frac{\partial f(E)}{\partial E} \right\|^{-1}$ queries to U



Error-corrected quantum chemistry simulation

Science 309:5741 (2005), 1704-1707, PRX 8, 041015 (2018), PRL 121, 010501 (2018)

1. Prepare an ansatz wavefunction ψ with “reasonable” support on the ground state

$$H |k\rangle = E_k |k\rangle \quad |\langle\psi|0\rangle|^2 = \text{not-too-small}$$

2. Form quantum circuit $U = e^{-if(H)}$ that encodes Hamiltonian spectrum in its eigenvalues

e.g., for
Qubitization: $f(H) = \arccos(H/\lambda) \quad U = e^{i \arccos(H/\lambda)}$

3. Application of U to ψ accumulates phases $f(E)$ encoding the spectrum

$$U |\psi\rangle = \sum_k \underbrace{\langle k|\psi\rangle}_{a_k} e^{-if(E_k)} |k\rangle$$

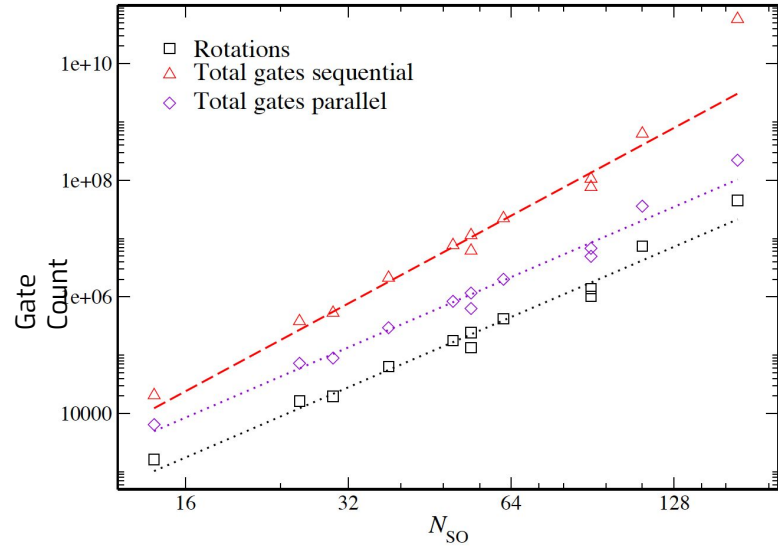
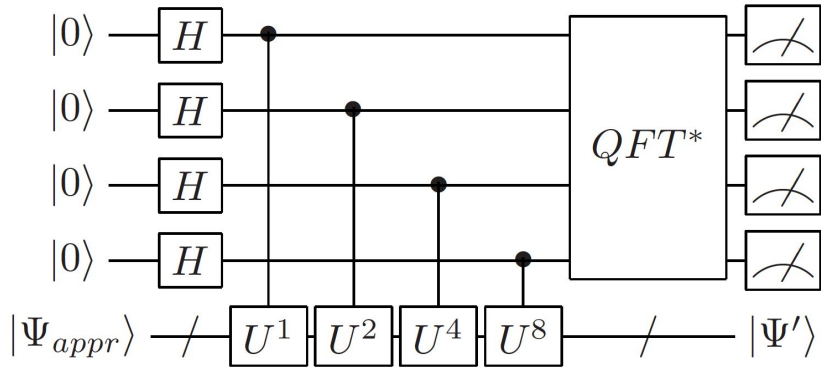
4. Phase estimation gives E_0 with error ϵ and probability $|a_0|^2$ using $\mathcal{O}\left(\frac{\lambda}{\epsilon}\right)$ queries to U



Simulating Quantum Mechanics on a Quantum Computer

Phase Estimation Algorithm

Time-evolution of eigenstate encodes the eigenvalues in phase information



$$T = \frac{\pi}{\epsilon} \approx 4000 E_h^{-1}$$

Very long coherence times required for eigenstate preparation

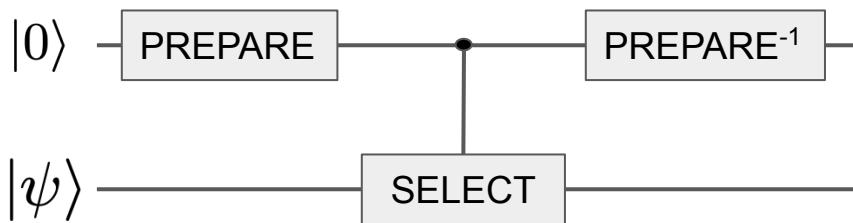
Block encoding via LCU

$$H = \sum_{\ell=1}^L \omega_{\ell} U_{\ell} \quad \lambda = \sum_{\ell=1}^L |\omega_{\ell}|$$

A linear combinations of unitaries representation

$$\text{SELECT } |\ell\rangle |\psi\rangle \mapsto |\ell\rangle U_{\ell} |\psi\rangle$$

$$\text{PREPARE } |0\rangle^{\otimes \log L} \mapsto \sum_{\ell=0}^{L-1} \sqrt{\frac{w_{\ell}}{\lambda}} |\ell\rangle$$



Block encoding H

$$U = \begin{bmatrix} \mathcal{H} & \sqrt{I - \mathcal{H}^2} \\ \sqrt{I - \mathcal{H}^2} & -\mathcal{H} \end{bmatrix}$$

$$= Z \otimes \mathcal{H} + X \otimes \sqrt{I - \mathcal{H}^2}$$

2D subspaces

$$\mathcal{H} = \sum_{\lambda} \lambda |\lambda\rangle \langle \lambda|$$

$$U|0\rangle|\lambda\rangle = \lambda|0\rangle|\lambda\rangle + \sqrt{1 - \lambda^2}|1\rangle|\lambda\rangle$$

$$U|1\rangle|\lambda\rangle = -\lambda|1\rangle|\lambda\rangle + \sqrt{1 - \lambda^2}|0\rangle|\lambda\rangle$$

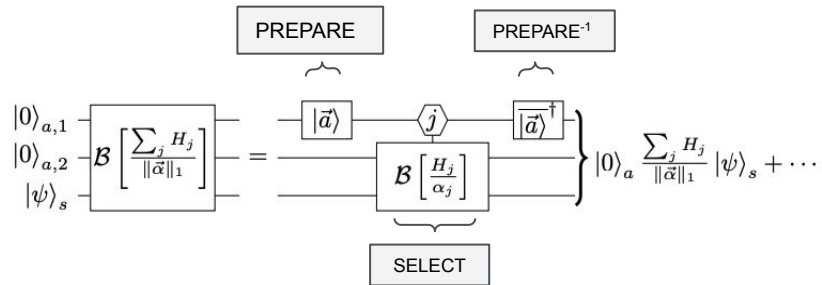
$$U = e^{i \cos^{-1}(\mathcal{H})}$$

block encodings arithmetic

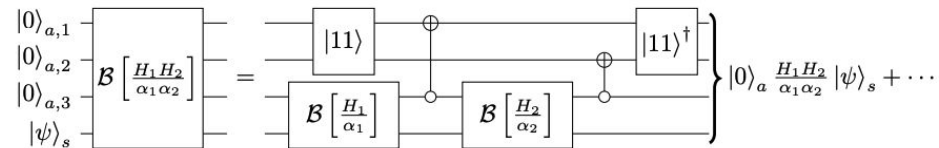
$$\mathcal{B}[H/\alpha] = \begin{pmatrix} H/\alpha & \cdots \\ \vdots & \ddots \end{pmatrix}$$

Given block encodings for H_1, H_2, \dots, H_m basic block encoding arithmetic allows you to generate a unitary encoding for any H in the algebra generated by H_1, H_2, \dots, H_m

Adding two block encodings



Multiplying two block encodings

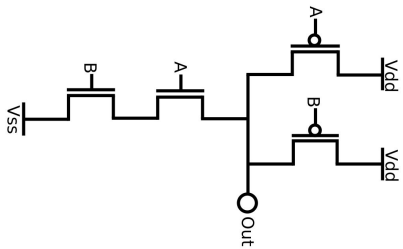
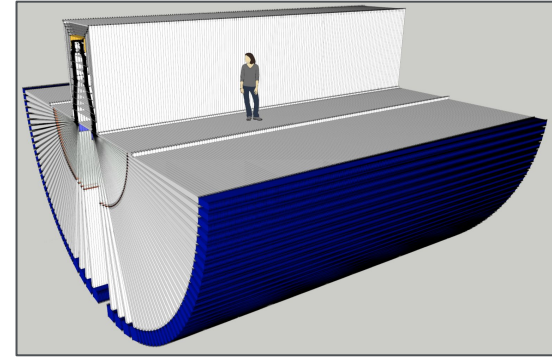


Space-time considerations are different within error-correction

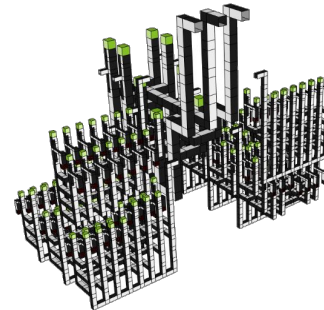
What we have in mind is a device with $>99.95\%$ fidelity physical gates and $\sim 1\text{MM}$ physical qubits

$\sim 1\text{k}$ “physical qubits” per “logical qubit”

- Certain necessary gates (e.g. Toffolis) are very slow, require hundreds of *logical qubits*
- Gives a huge “constant factor slowdown” in spacetime versus classical computers



classical NAND gate (CMOS)
 $<10^{-9}$ “transistorseconds”

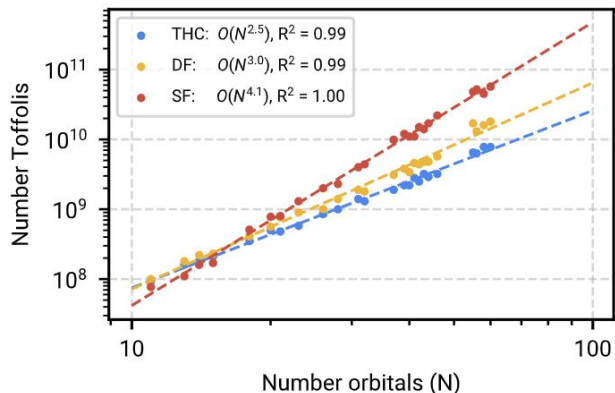
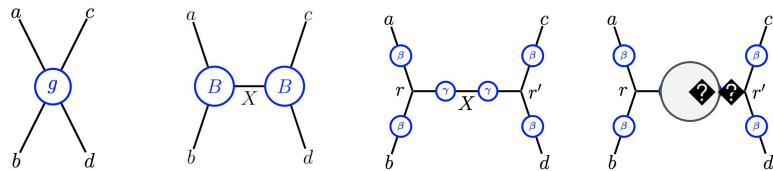


“quantum NAND” gate
 (distillation of Toffoli state)
 >10 “qubitseconds”

Cost of qubitization: block encodings

The complexity of building SELECT and PREPARE largely depends on the Hamiltonian factorization we use. The Coulomb kernel can be factorized in many different ways

$$H = \sum_{abcd} h_{abcd} a_a^\dagger a_b^\dagger a_d a_c = \sum_{\ell=0}^{L-1} \omega_\ell U_\ell$$

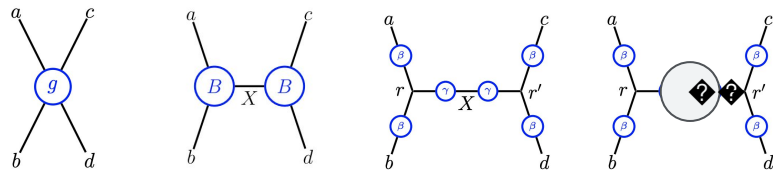


Qubits	$\tilde{O}(N^2)$	$\tilde{O}(N^{3/2})$	$\tilde{O}(N\sqrt{\Xi})$	$\tilde{O}(N)$
Toffoli	$\tilde{O}(N^2\lambda/\epsilon)$	$\tilde{O}(N^{3/2}\lambda/\epsilon)$	$\tilde{O}(N\lambda\sqrt{\Xi}/\epsilon)$	$\tilde{O}(N\lambda/\epsilon)$
Qubits	$\tilde{O}(N_k^{3/2}N^2)$	$\tilde{O}(N_k N^{3/2})$	$\tilde{O}(\sqrt{N_k}N\sqrt{\Xi})$	$\tilde{O}(N_k N)$
Toffoli	$\tilde{O}(N_k^{3/2}N^2\lambda_{\text{sparse}}/\epsilon)$	$\tilde{O}(N_k N^{3/2}\lambda_{\text{SF}}/\epsilon)$	$\tilde{O}(\sqrt{N_k}N\sqrt{\Xi}\lambda_{\text{DF}}/\epsilon)$	$\tilde{O}(N_k N\lambda_{\text{DF}}/\epsilon)$

Cost of qubitization: block encodings

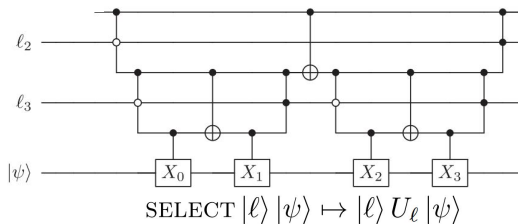
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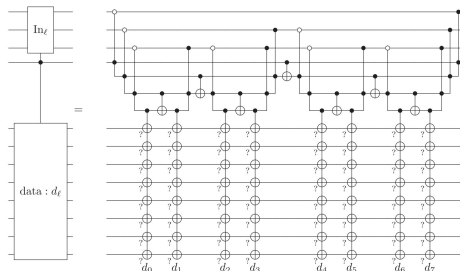


Important primitives to construct block encodings

For loop on a seg-tree **O(L) Toffoli**



Q-ROM **O(L) Toffoli + log(L) ancilla** or **O((Lβ)^{0.5}) Toffoli + O((Lβ)^{0.5}) ancilla**

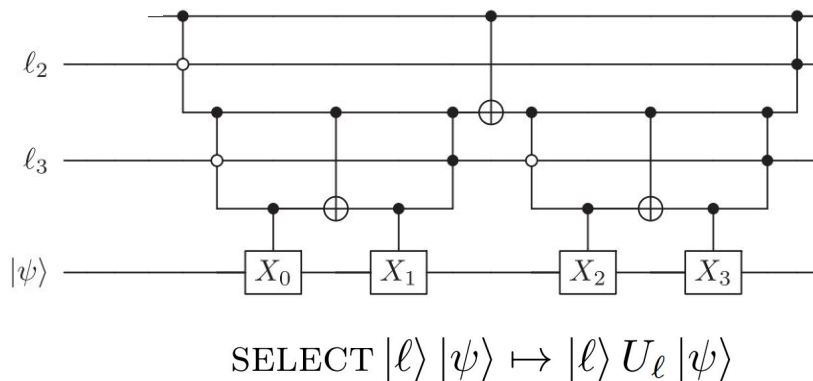
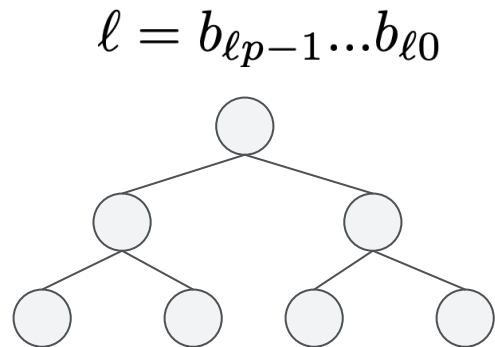


State preparation: **PREPARE O(L^{1/2}) cost**

$$\sqrt{\frac{1}{L}} \sum_{\ell=0}^{L-1} |\ell\rangle |0\rangle \quad \text{QROM} \quad \sum_{\ell=0}^{L-1} \sqrt{\frac{\omega_\ell}{\lambda}} |\ell\rangle |\text{junk}_\ell\rangle$$

Interlude: Circuit gadgets: for loop

Main idea: perform loop by doing depth-first-search on a binary tree

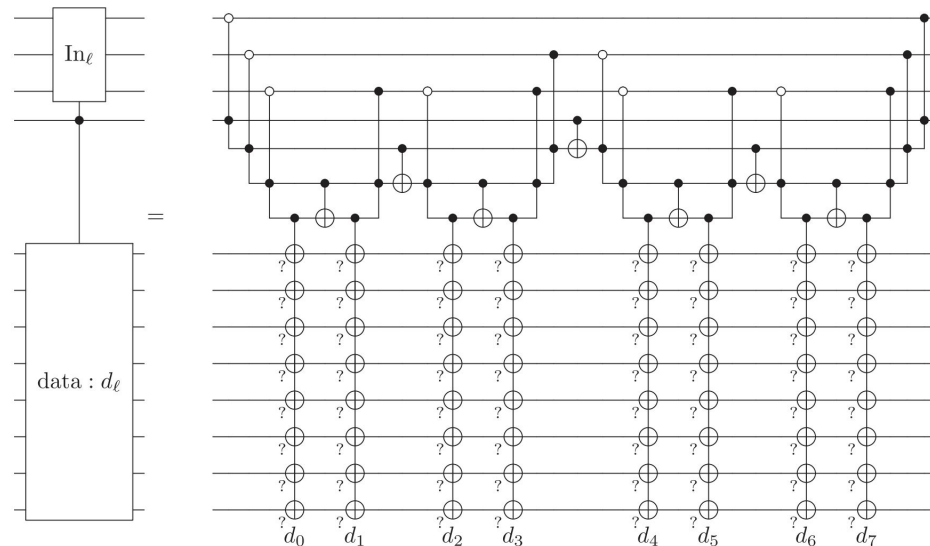
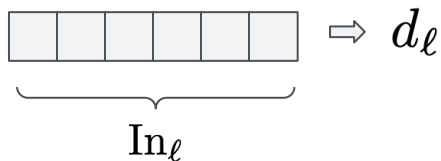


$O(L)$ Toffoli complexity to construct tree and $O(\log(L))$ qubits for control

Interlude: Circuit gadgets: Data lookup + multiplex

Main idea: read-only-memory circuit using unary iteration

$$D|In_\ell\rangle|0_{0\dots 0_d}\rangle = |In_\ell\rangle|d_\ell\rangle$$



$O(L)$ Toffoli + $\log(L)$ ancilla

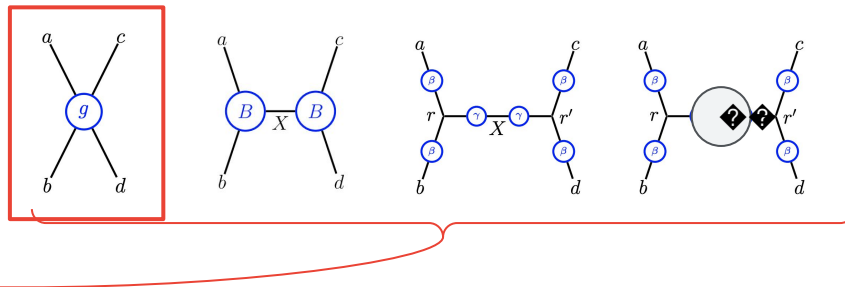
or

$O((L\beta)^{0.5})$ Toffoli + $O((L\beta)^{0.5})$ ancilla

Cost of qubitization: block encodings

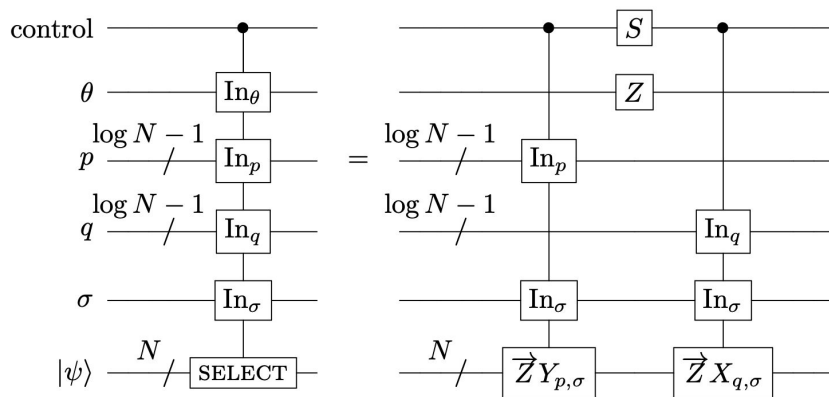
The complexity of building SELECT and PREPARE largely depends on the Hamiltonian factorization we use. The Coulomb kernel can be factorized in many different ways

$$H = \sum_{abcd} h_{abcd} a_a^\dagger a_b^\dagger a_d a_c = \sum_{\ell=0}^{L-1} \omega_\ell U_\ell$$



$$V' = \frac{1}{8} \sum_{\alpha, \beta \in \{\uparrow, \downarrow\}} \sum_{p, q, r, s=1}^{N/2} V_{pqrs} Q_{pq\alpha} Q_{rs\beta}$$

$$Q_{pq\sigma} = \begin{cases} X_{p,\sigma} \vec{Z} X_{q,\sigma}, & p < q, \\ Y_{p,\sigma} \vec{Z} Y_{q,\sigma}, & p > q, \\ -Z_{p,\sigma}, & p = q. \end{cases}$$

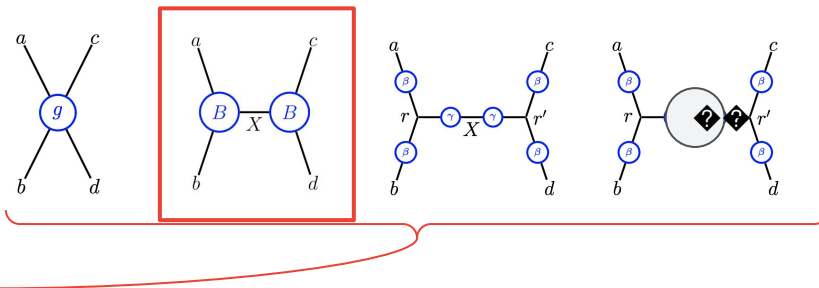


O(N)

Cost of qubitization: block encodings

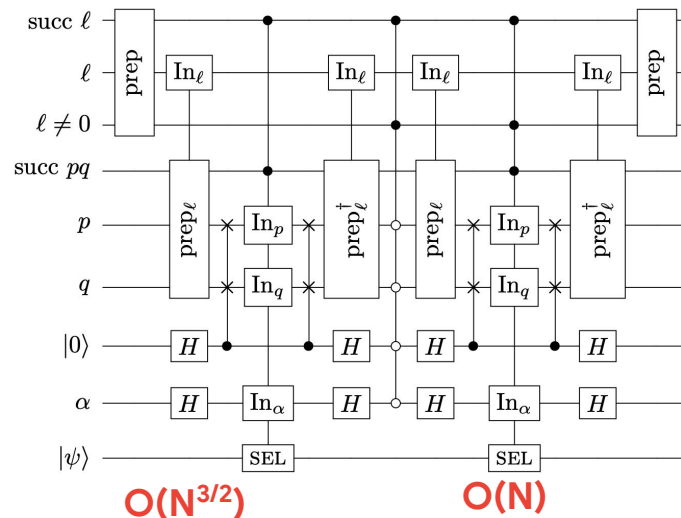
The complexity of building SELECT and PREPARE largely depends on the Hamiltonian factorization we use. The Coulomb kernel can be factorized in many different ways

$$H = \sum_{abcd} h_{abcd} a_a^\dagger a_b^\dagger a_d a_c = \sum_{\ell=0}^{L-1} \omega_\ell U_\ell$$



$$\frac{1}{8} \sum_{\ell=1}^L \left(\sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{p, q=1}^{N/2} W_{pq}^{(\ell)} Q_{pq\sigma} \right)^2$$

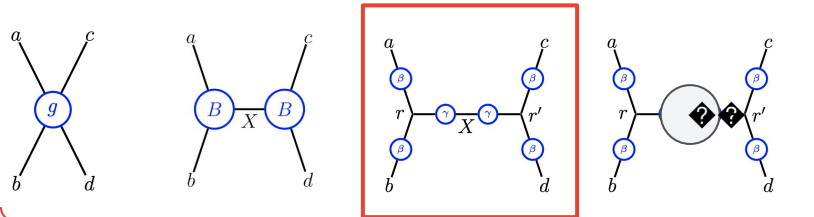
$$Q_{pq\sigma} = \begin{cases} X_{p,\sigma} \vec{Z} X_{q,\sigma}, & p < q, \\ Y_{p,\sigma} \vec{Z} Y_{q,\sigma}, & p > q, \\ -Z_{p,\sigma}, & p = q. \end{cases}$$



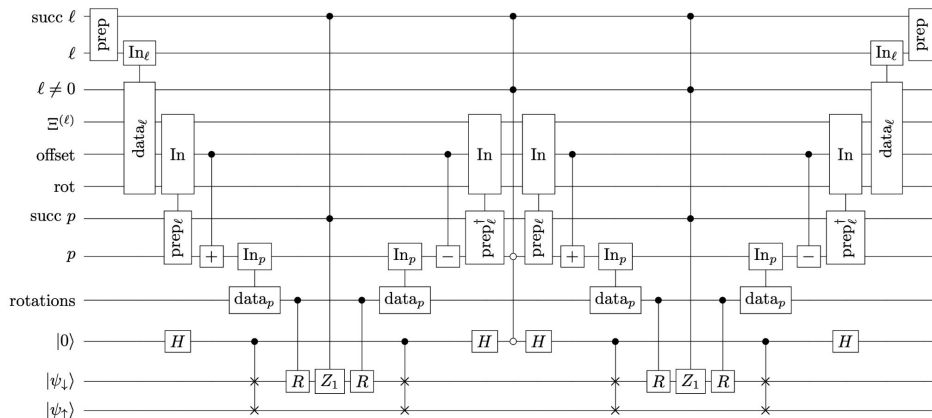
Cost of qubitization: block encodings

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$$\frac{1}{8} \sum_{\ell=1}^L U_\ell \left(\sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{p=1}^{N/2} f_p^{(\ell)} (\mathbb{1} - Z_{p,\sigma}) \right)^2 U_\ell^\dagger$$

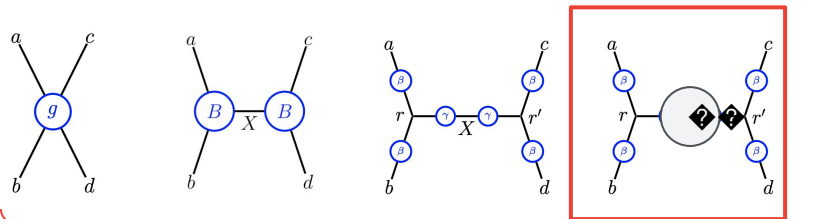


$O(N\epsilon^{1/2})$

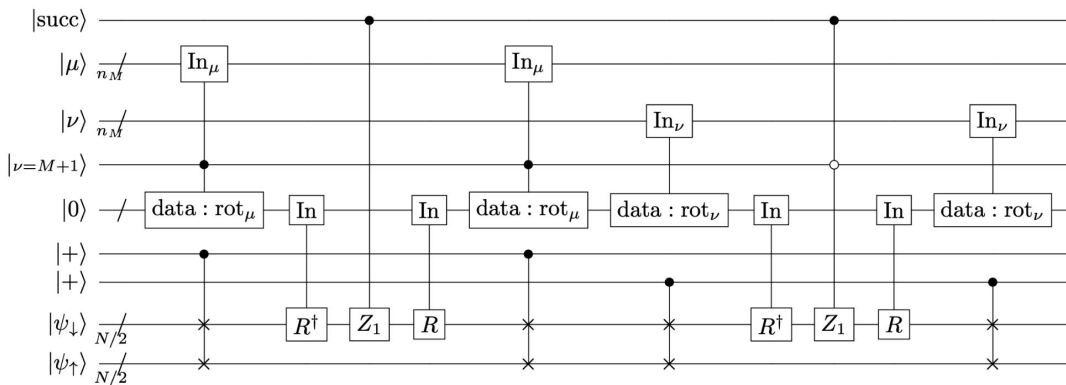
Cost of qubitization: block encodings

The complexity of building SELECT and PREPARE largely depends on the Hamiltonian factorization we use. The Coulomb kernel can be factorized in many different ways

$$H = \sum_{abcd} h_{abcd} a_a^\dagger a_b^\dagger a_d a_c = \sum_{\ell=0}^{L-1} \omega_\ell U_\ell$$



$$\frac{1}{8} \sum_{\alpha, \beta \in \{\uparrow, \downarrow\}} \sum_{\mu, \nu=1}^M \zeta_{\mu\nu} U_\mu^\dagger Z_{1,\alpha} U_\mu U_\nu^\dagger Z_{1,\beta} U_\nu$$

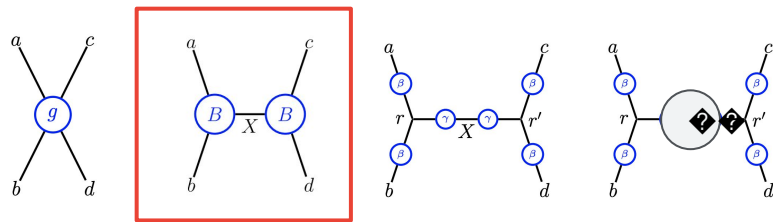


$O(N)$

Coulomb tensor factorizations symmetry-adapted

Each tensor factorization know must be constrained to the appropriate momentum conservation sum-rule.

$$H_2 = \frac{1}{2} \sum_{\sigma, \tau} \sum_{\mathbf{Q}, \mathbf{k}, \mathbf{k}'} \sum_{pqrs} V_{p\mathbf{k}, q(\mathbf{k} \ominus \mathbf{Q}), r(\mathbf{k}' \ominus \mathbf{Q}), s\mathbf{k}'} a_{p\mathbf{k}\sigma}^\dagger a_{q(\mathbf{k} \ominus \mathbf{Q})\sigma} a_{r(\mathbf{k}' \ominus \mathbf{Q})\tau}^\dagger a_{s\mathbf{k}'\tau}$$

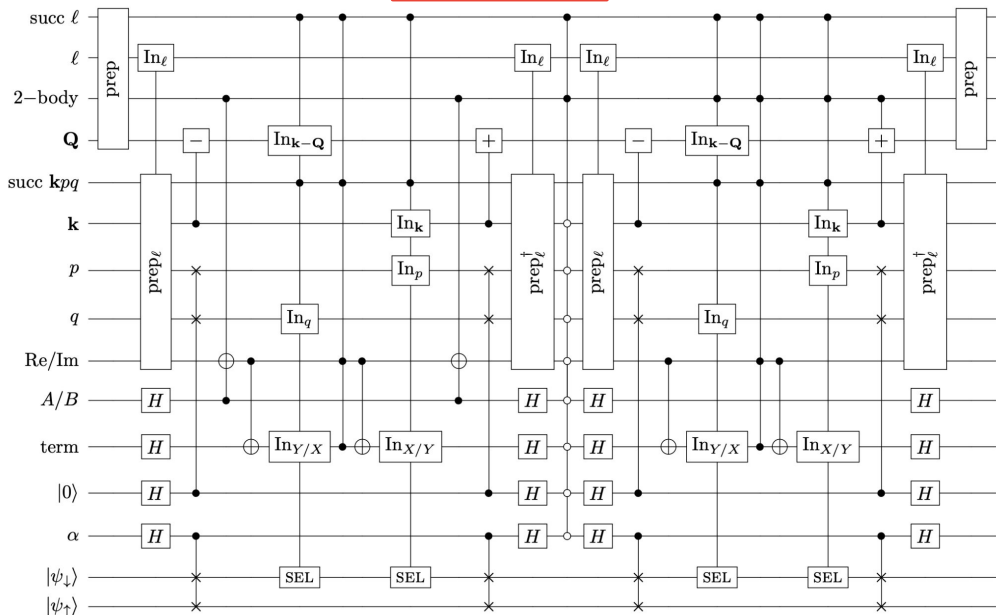


$$\hat{H}'_2 = \frac{1}{2} \sum_{\mathbf{Q}} \sum_n^{N_k} \sum_n^M \left(\hat{A}_n^2(\mathbf{Q}) + \hat{B}_n^2(\mathbf{Q}) \right)$$

A and B terms have familiar Majorana fermion operator representations!

$$\hat{A}_n(\mathbf{Q} \neq 0) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{\mathbf{k}}^{N_k} \sum_{pq}^{N/2} \left(\frac{i\text{Re}[L_{pkq(\mathbf{k} \ominus \mathbf{Q}), n}]}{4} \left(\bar{Z}X_{p\mathbf{k}\sigma} \bar{Z}Y_{q(\mathbf{k} \ominus \mathbf{Q})\sigma} - \bar{Z}Y_{p\mathbf{k}\sigma} \bar{Z}X_{q(\mathbf{k} \ominus \mathbf{Q})\sigma} \right) \right. \\ \left. + \frac{i\text{Im}[L_{pkq(\mathbf{k} \ominus \mathbf{Q}), n}]}{4} \left(\bar{Z}X_{p\mathbf{k}\sigma} \bar{Z}X_{q(\mathbf{k} \ominus \mathbf{Q})\sigma} + \bar{Z}Y_{p\mathbf{k}\sigma} \bar{Z}Y_{q(\mathbf{k} \ominus \mathbf{Q})\sigma} \right) \right)$$

$O(N_k^2 N^2)$ vs $O(N_k N^2)$

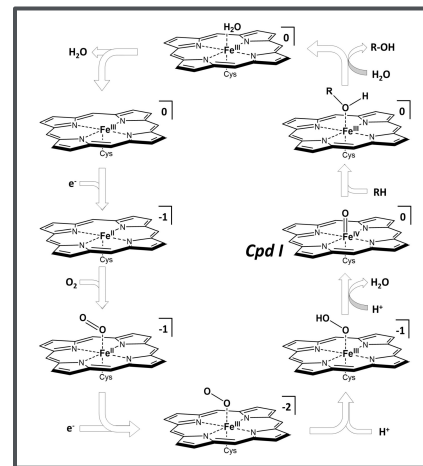
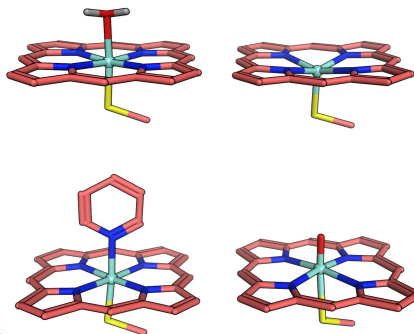
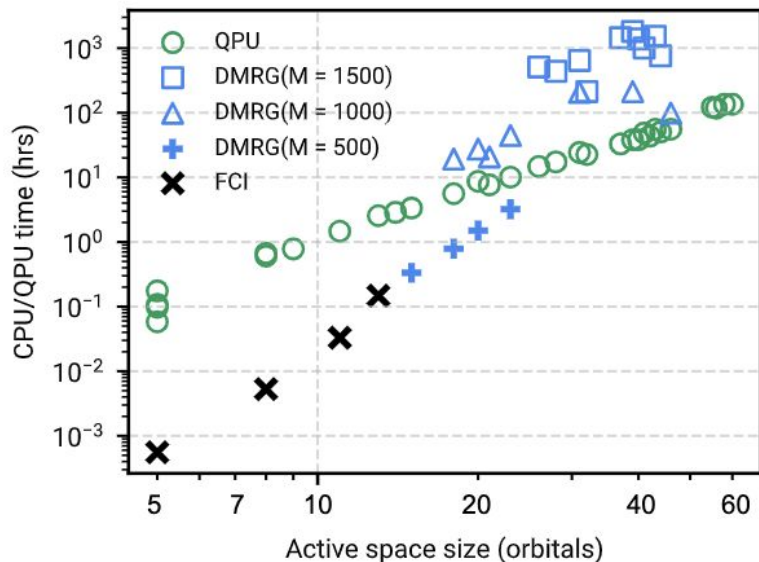


Assessing quantum/classical boundary for P450

PNAS 119 (38), 2203533119 (2022)

Critical to articulate more specific industry-relevant use cases

P450 is strongly correlated iron-porphyrin / drug anti-target



We observe onset of quantum advantage for active space sizes near 80 qubits

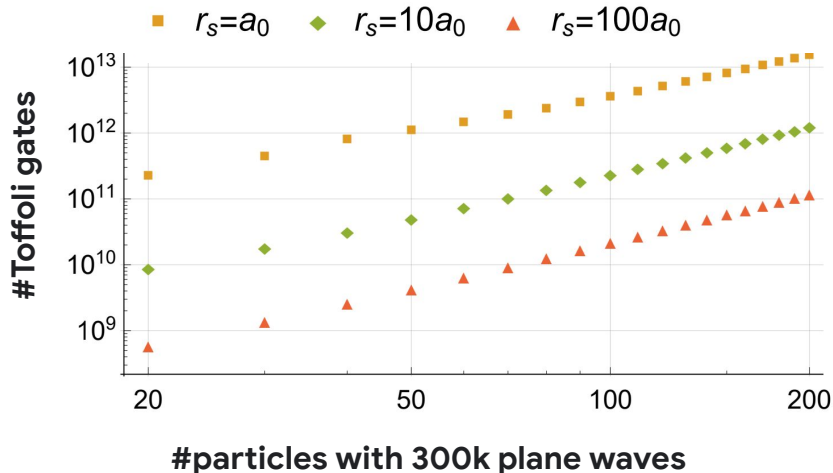
Calculations would require a few million physical qubits assuming $1e-4$ error rates in surface code

The future of chemistry is 1st quantized!

~100X more plane waves than molecular orbitals needed for target precision
In 2nd quantization #qubits = #orbitals so it is critical to use molecular orbitals



In 1st quantization #qubits = (#particles) log (#orbitals) but algorithmically challenging
Nature QI 5, 92 gives 1st quantized plane wave algorithm scaling as $(\text{\#particles})^{8/3}(\text{\#orbitals})^{1/3}$



PRX Quantum 2, 040332 (2021) compiles first quantized chem algorithms to fault-tolerant gates

Enables accurate simulation of realistic materials!

Non-Born-Oppenheimer quantum dynamics is now possible, and with very little overhead!

The future of chemistry is 1st quantized!

$$T = \sum_{i=1}^{\eta} \sum_{\mathbf{p} \in \mathcal{G}} \frac{\|\mathbf{G}_{\mathbf{p}}\|^2}{2} |\mathbf{p}\rangle \langle \mathbf{p}|_i$$

$$U = -\frac{4\pi}{\Omega} \sum_{i=1}^{\eta} \sum_{\mathbf{q} \in \mathcal{G}} \sum_{\substack{\nu \in \mathcal{G}_0 \\ (\mathbf{q}-\nu) \in \mathcal{G}}} \frac{\sum_{I=1}^L Z_I e^{i\mathbf{G}_{\nu} \cdot \mathbf{R}_I}}{\|\mathbf{G}_{\nu}\|^2} |\mathbf{q} - \nu\rangle \langle \mathbf{q}|_i$$

$$V = \frac{2\pi}{\Omega} \sum_{i \neq j}^{\eta} \sum_{\mathbf{p}, \mathbf{q} \in \mathcal{G}} \sum_{\substack{\nu \in \mathcal{G}_0 \\ (\mathbf{p}+\nu) \in \mathcal{G} \\ (\mathbf{q}-\nu) \in \mathcal{G}}} \frac{1}{\|\mathbf{G}_{\nu}\|^2} |\mathbf{p} + \nu\rangle \langle \mathbf{p}|_i |\mathbf{q} - \nu\rangle \langle \mathbf{q}|_j$$

$$|0\rangle \text{ --- } \boxed{R_y(\theta)} \text{ --- } (\cos(\theta) |0\rangle + \sin(\theta) |1\rangle)_a$$

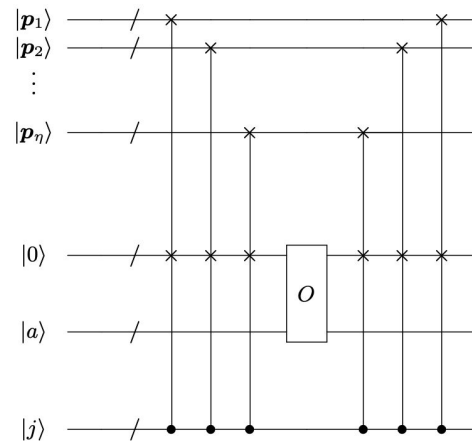
$$|0\rangle \text{ --- } \boxed{R_y(\arccos \theta_{\lambda})} \text{ --- } \left(\sqrt{\frac{\lambda_U}{\lambda_U + \lambda_V}} |0\rangle + \sqrt{\frac{\lambda_V}{\lambda_U + \lambda_V}} |1\rangle \right)_m$$

$$|0\rangle \text{ --- } \boxed{\text{PREP}_T} \text{ --- } \text{Eq. (89)}$$

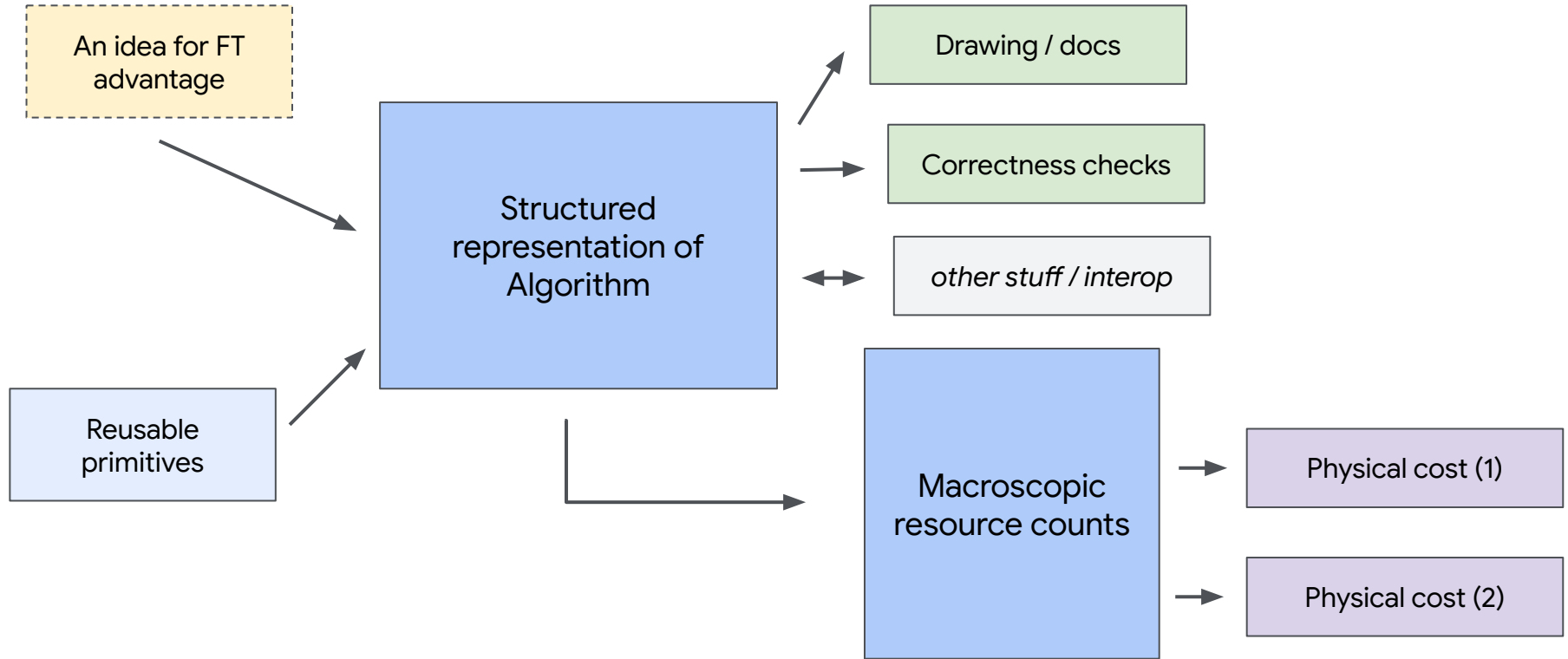
$$|0\rangle \text{ --- } \boxed{\text{extra PREP}_V} \text{ --- } \sum_{j=1}^{\eta} |j\rangle_e |i \stackrel{?}{=} j\rangle_c$$

$$|0\rangle \text{ --- } \boxed{\text{Momentum state}} \text{ --- } \sqrt{\frac{P_{\nu}}{\lambda_{\nu}}} |0\rangle_j \sum_{\nu \in \mathcal{G}_0} \frac{1}{\|\nu\|} |\nu\rangle_k + |\perp\rangle$$

$$|0\rangle \text{ --- } \boxed{\text{QROM}} \text{ --- } \frac{1}{\sqrt{\lambda_Z}} \sum_{I=1}^L \sqrt{Z_I} |\mathbf{R}_I\rangle_l$$



We need new software tools for this work

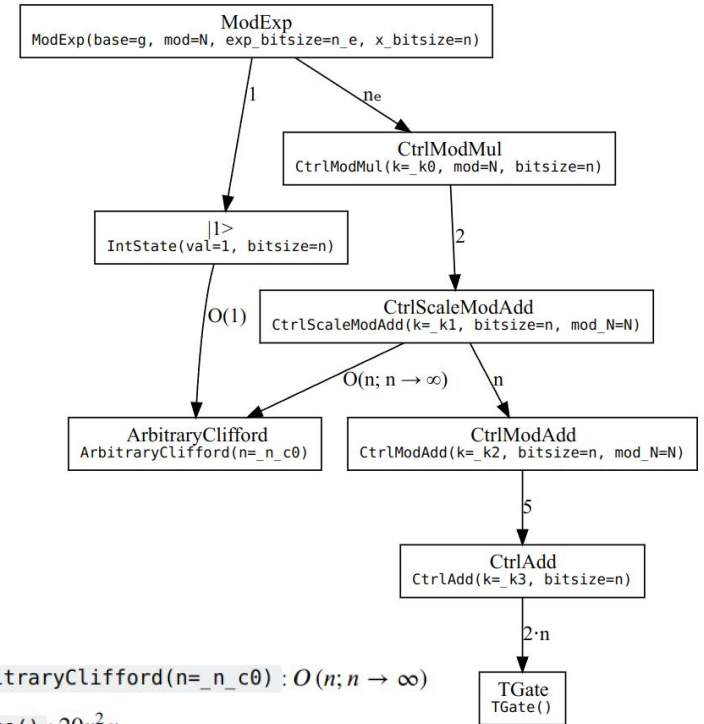
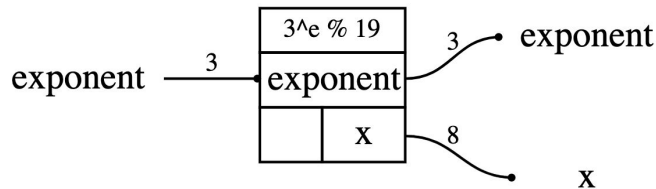


Bloqs: Structured Representation of Algos

We can't execute these algorithms (yet), so no requirement to code everything "all the way down"

Allow users to freely annotate known quantities and write protocols to query properties for complex algorithms.

E.g.: drawing, testing classical-reversible subroutines, counting resources etc.



ArbitraryClifford($n = n_c0$) : $O(n; n \rightarrow \infty)$

TGate() : $20n^2 n_e$

Cirq-FT: Cirq for Fault Tolerant algorithms

Make it easier to write Fault Tolerant algorithms in Cirq using qubit registers, quantum memory management etc.

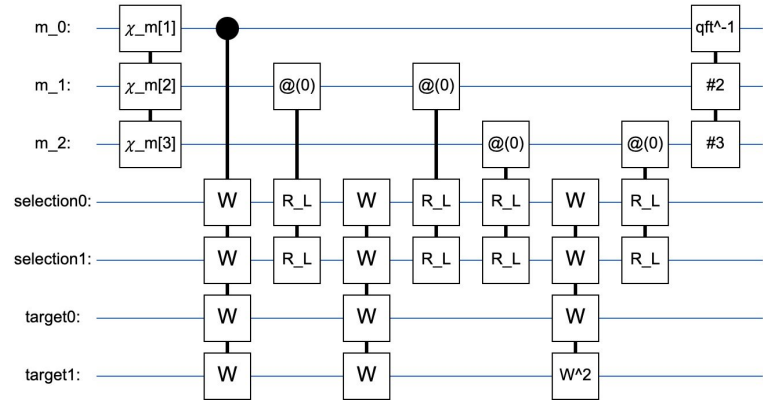
Reusable library of primitives and Bi-Directional Interop with Bloqs

Efficient resource counting for large systems.

```
@frozen
class MultiTargetCSwap(GateWithRegisters):
    bitsize: int

    @cached_property
    def registers(self) -> Registers:
        return Registers.build(ctrl=1, x=self.bitsize, y=self.bitsize)

    def decompose_from_registers(self,
        ctrl: Sequence[cirq.Qid],
        x: Sequence[cirq.Qid],
        y: Sequence[cirq.Qid],
    ) -> cirq.OP_TREE:
        yield [cirq.CSWAP(*ctrl, t_x, t_y) for t_x, t_y in zip(x, y)]
```

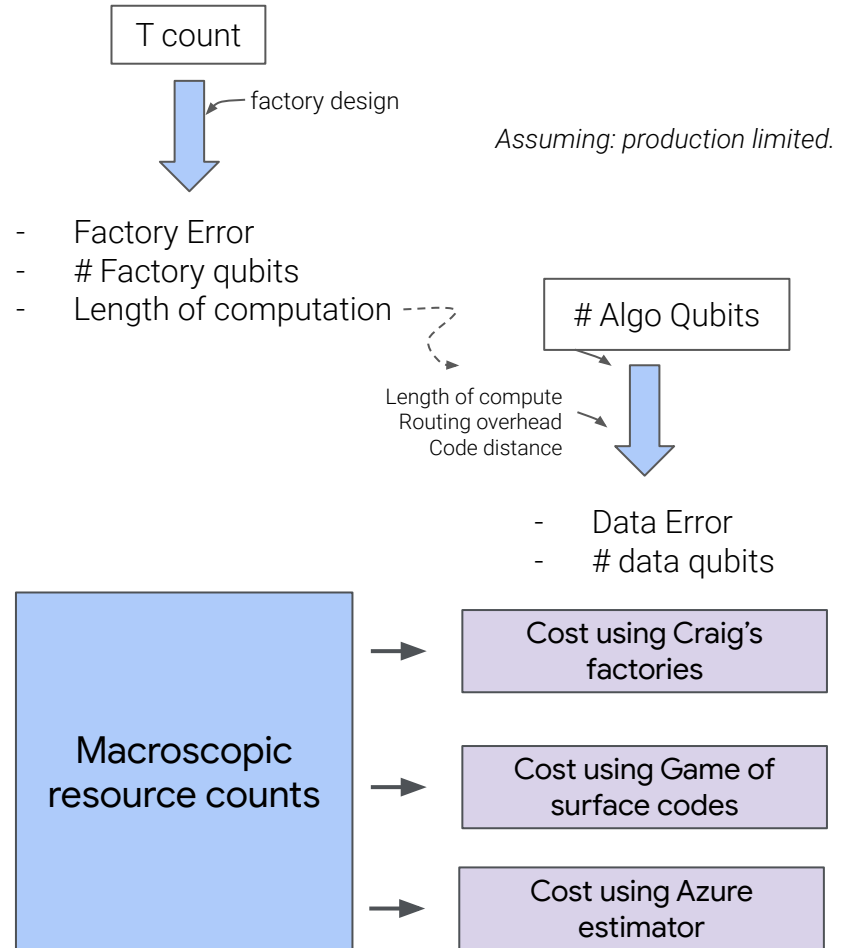


Physical Costing

Formulas exist for estimating wallclock time, # physical qubits given T-gate count, code distance, etc.

They can be inaccessible or indiscriminately applied

Goal: put a variety of them in one place with a common interface.



Thank you!



Quantum AI

- Google has PhD intern programs / student stay programs
- Interest in collaborating on FT algorithms applications in challenging domains
- Interest in quantum many-body methods development

