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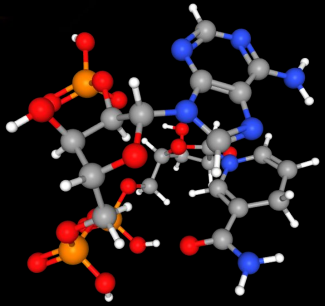
Quantum chemistry on the Sycamore quantum processor

Ryan Babbush
February 2020



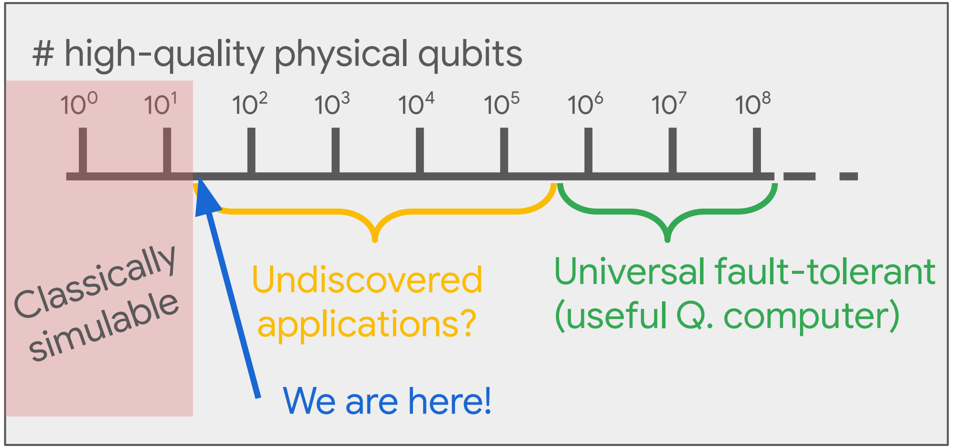
Quantum computers today

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

Last year, Google team demonstrated “quantum supremacy”
i.e., we used our 54 qubit quantum computer to perform a well defined computational task that would be intractable on a classical computer

Ultimate goal is quantum error-correction
Has very large resource overheads

We’ll have NISQ devices in the meantime
Will we be able to use such devices to achieve quantum supremacy on a useful application?



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The molecular electronic structure problem

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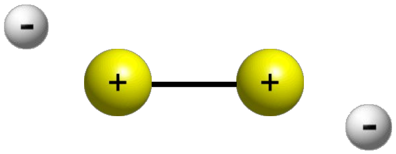
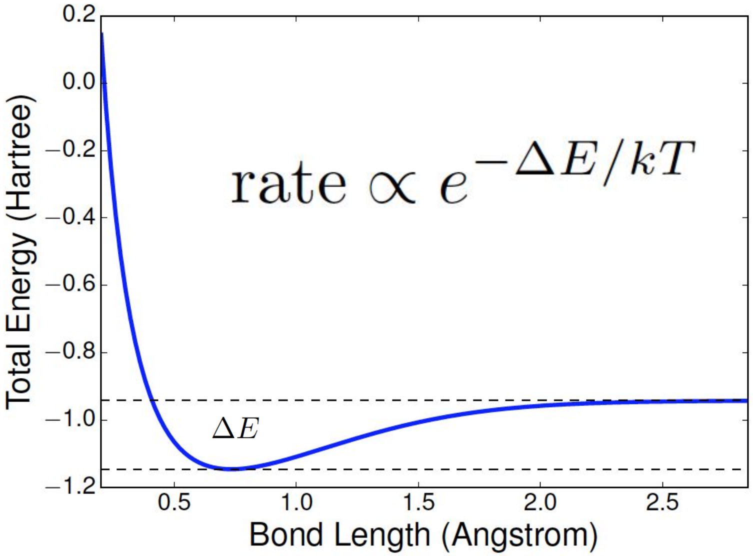


Goal is to solve for the energy of molecule

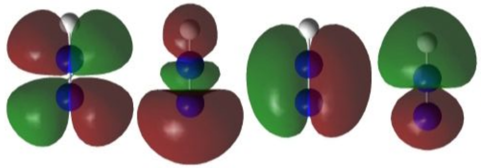
$$H = \hat{T}_{\text{nuc}} + \hat{T}_{\text{elec}} + \hat{V}_{\text{nuc-nuc}} + \hat{V}_{\text{nuc-elec}} + \hat{V}_{\text{elec-elec}}$$

Energy surfaces allow us to understand reactions
Need chemical accuracy (1 kcal/mol) for rates



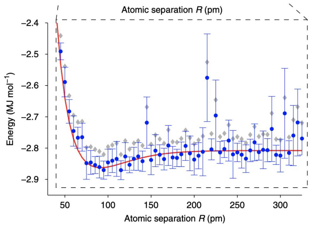
Such accuracy is often classically intractable
Especially for systems with strong correlation

To represent wavefunctions on computer one must discretize space (confine to basis)

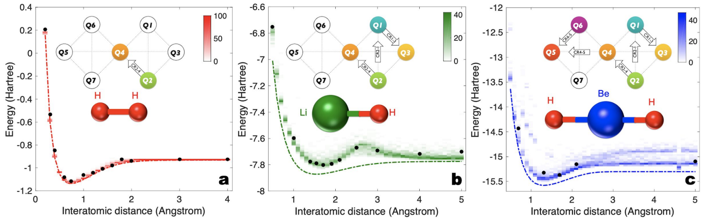


$$a_1\,|0011\rangle + a_2\,|0101\rangle + a_3\,|1001\rangle + a_4\,|0110\rangle + a_5\,|1010\rangle + a_6\,|1100\rangle$$

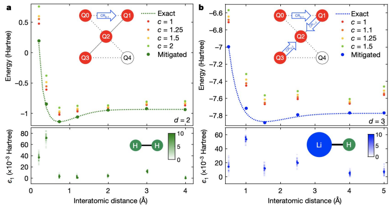
Everybody loves applying VQE to chemistry



O'Malley, Babbush, et al. (2016)



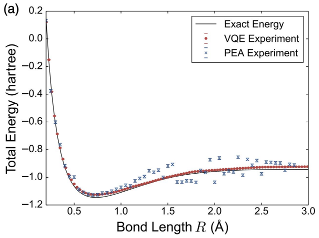
Hempel et al. (2018)



2014

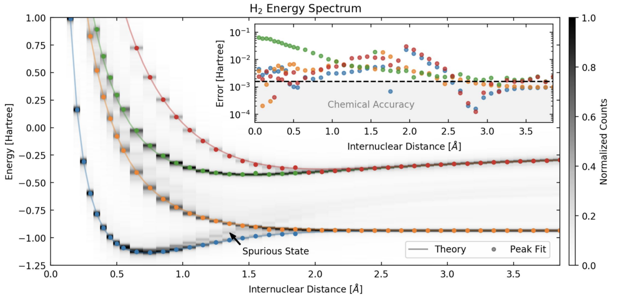
Present

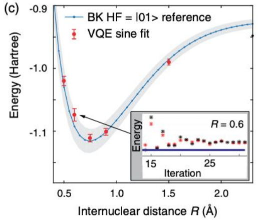
Peruzzo, McClean, et al. (2014)



Kandala et al. (2017)

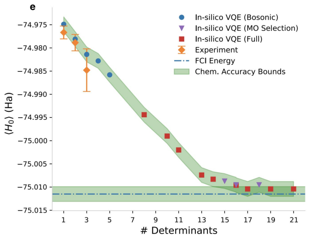
Colless et al. (2017)





Kandala et al. (2019),

Nam et al. (2019)



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Why perform these experiments at all?

- WAY easier to publish in Nature than serious theory work (bad reason)
- Forces algorithmists to feel the pain of a real experiment!
- Provides a holistic device-level benchmark in the context of an actual algorithm
  - Where is our device relative to competitors?
  - Exactly how far are we really from something classically intractable?
- Study the effects of noise on algorithm / test error-mitigation ideas

Hartree-Fock on a quantum computer

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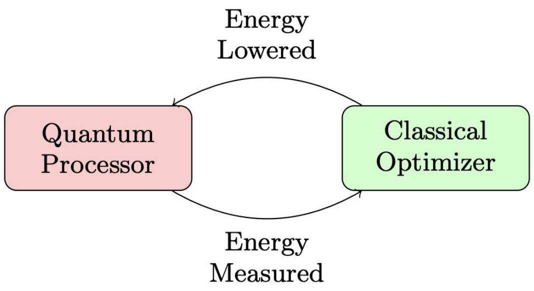
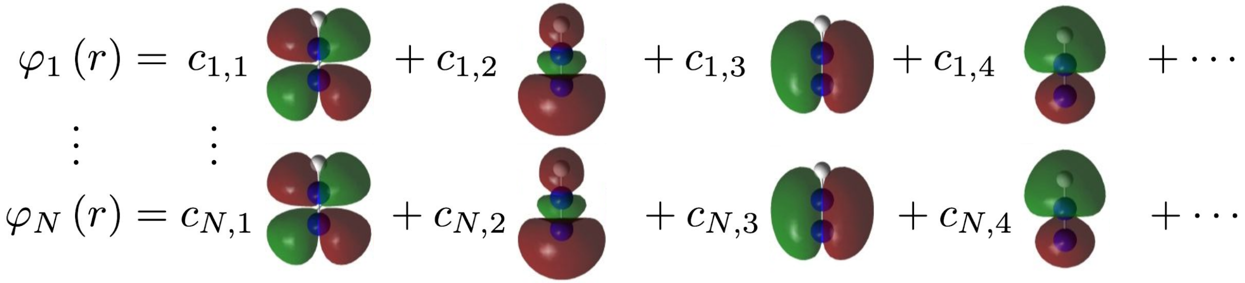


Our ansatz corresponds to an orbital (basis) rotation



simple circuit with linear depth complexity

$$|\psi(\kappa)\rangle = \exp\left[-\sum_{pq} \kappa_{pq} a_p^\dagger a_q\right] |\phi\rangle \qquad c_{pq} = [\log \kappa]_{pq}$$

Optimizing over these parameters solves for the lowest energy mean-field wavefunction (i.e., Hartree-Fock)

$$\min_{\kappa} \langle\phi| \underbrace{U_\kappa H U_\kappa^\dagger}_{H(\kappa)} |\phi\rangle$$

it's classically tractable - so why do it?

- Basis rotations are a ubiquitous primitive!
  - Optimal compilation known
  - Great benchmark!
- Very entangled state with tractable structure
  - Allows us to better understand errors
  - Structure simplifies implementation

Why the obsession with basis rotations?

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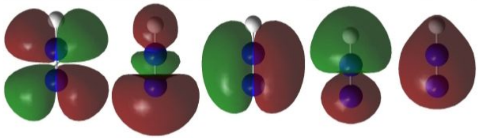
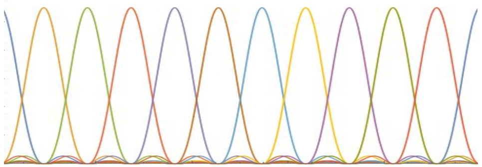
Using molecular orbitals leads to Hamiltonian with O(N^4) terms



$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

By changing the basis, we obtain Hamiltonian with O(N^2) terms - PRX 8, 011044 (2018)



$$H = \sum_{pq} V_{pq} n_p n_q + \underbrace{\sum_{pq} T_{pq} a_p^\dagger a_q}_{U\left(\sum_p \tau_p n_p\right) U^\dagger} \qquad n_p = a_p^\dagger a_p$$

Or we can factorize Hamiltonian into L = O(N) different bases - arXiv:1812.00954

$$H = U_0 \left(\sum_p g_p n_p \right) U_0^\dagger + \sum_{\ell=1}^{L} U_\ell \left(\sum_{pq} g_{pq}^{(\ell)} n_p n_q \right) U_\ell^\dagger$$

This form also helpful for estimating <H> while mitigating errors - arXiv:1907.13117

Optimal synthesis of basis rotation circuit

Physical Review Letters 120 (11), 110501 (2018)

$$|\psi(\vec{\kappa})\rangle = \exp\left[-\sum_{pq} \kappa_{pq} a_p^\dagger a_q\right] |\phi\rangle$$

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Physical Review Letters 120 (11), 110501 (2018)

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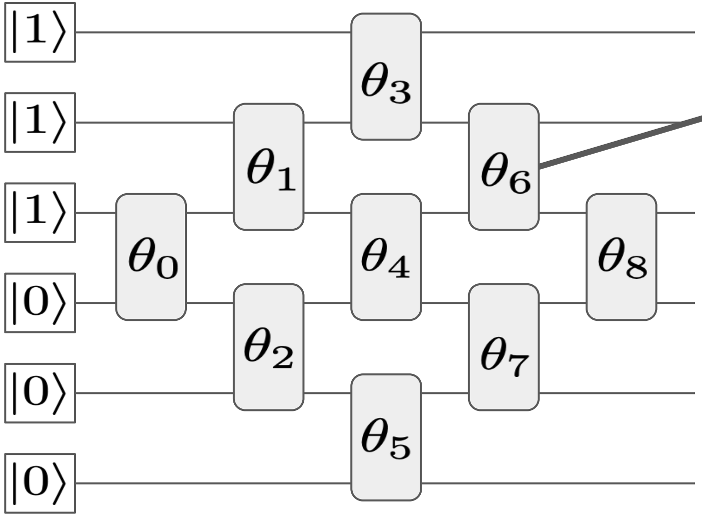
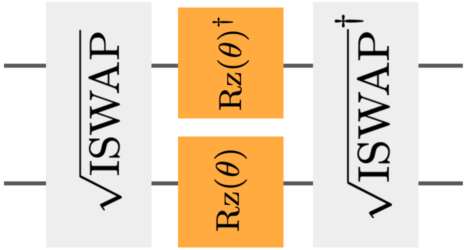


$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) & 0 \\ 0 & \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$G(\theta) =$



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Exploiting RDM structure for fewer errors / measurements

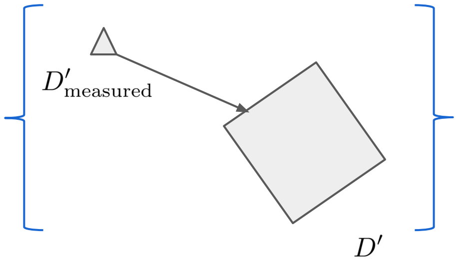
Simple energy evaluation and error-mitigation from Reduced Density Matrices (RDMs)

$$\langle H \rangle = \sum_{pq} h_{pq} \underbrace{\langle a_p^\dagger a_q \rangle}_{D'_{pq}} + \frac{1}{2} \sum_{pqrs} h_{pqrs} \underbrace{\langle a_p^\dagger a_q^\dagger a_r a_s \rangle}_{D''_{pqrs}}$$

$$D''_{pqrs} = \frac{1}{2} \left(D'_{ps} D'_{qr} - D'_{qs} D'_{pr} \right)$$

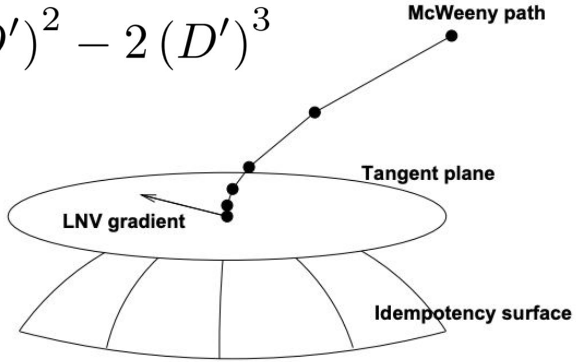
Hartree-Fock RDMs have known geometry

$$\left\{ \begin{aligned} \mathrm{Tr}\left[D'\right] &= n_{\text{electrons}} \\ D' &= \left(D'\right)^2 \\ D' &\succeq 0 \end{aligned} \right\} \equiv$$



Idempotency by engineered fixed points

$$D' = 3\left(D'\right)^2 - 2\left(D'\right)^3$$



Even general 2-RDMs have nontrivial structure which we can leverage for error-mitigation

New Journal of Physics 20 (5), 053020 (2018)

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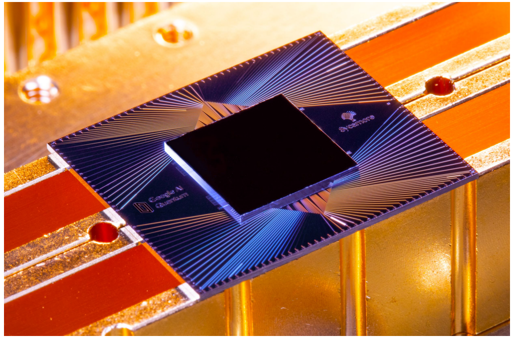
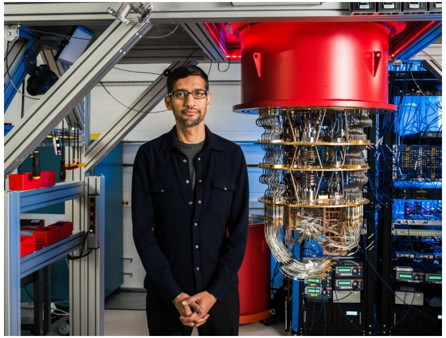
Google Sycamore superconducting qubit platform

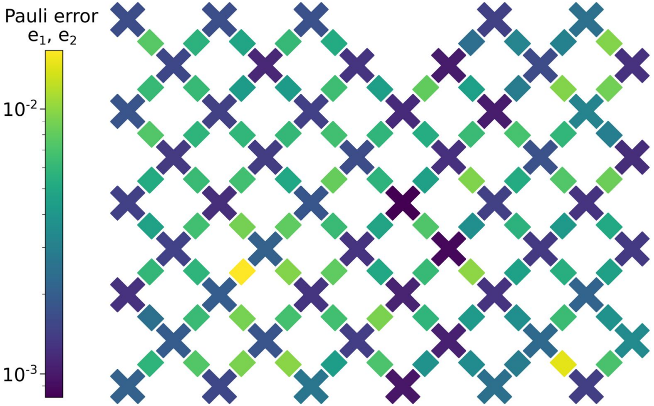
Sycamore platform has 54 planar transmon qubits tunably coupled in square lattice array





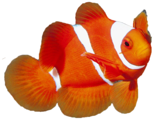
Pauli and measurement errors

Average error	Isolated	Simultaneous
Single-qubit (e_1)	0.15%	0.16%
Two-qubit (e_2)	0.36%	0.62%
Two-qubit, cycle (e_{2c})	0.65%	0.93%
Readout (e_r)	3.1%	3.8%



We collected *most* data through cloud interface

Cirq + OpenFermion



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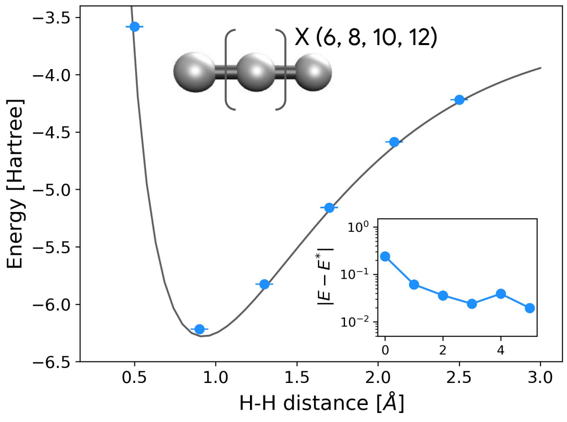
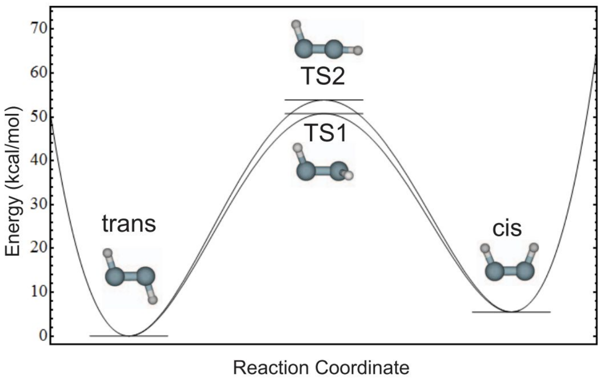
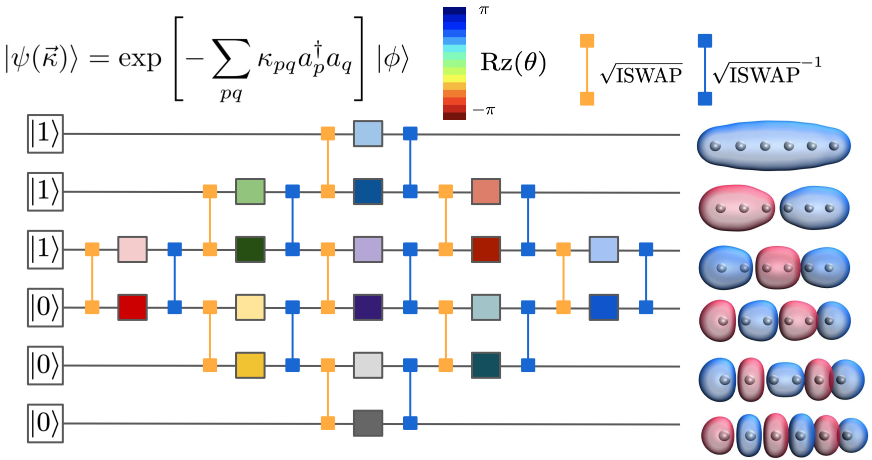
So how well does the machine do?

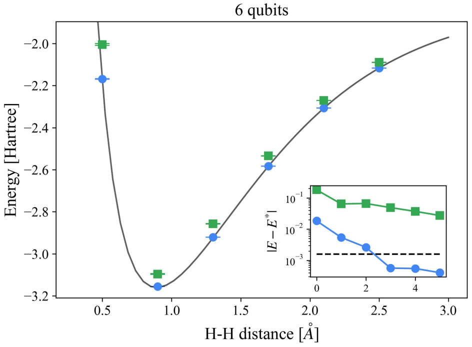




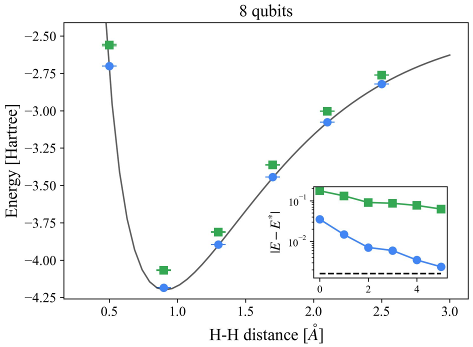
Hydrogen chain to benchmark out device



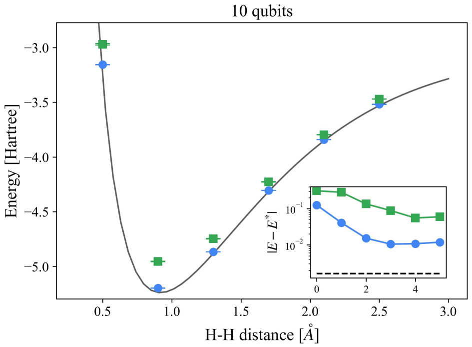
18 sqrt(iswap), 27 Rz



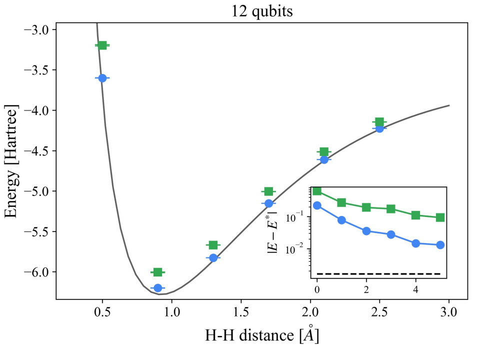
32 sqrt(iswap), 48 Rz



50 sqrt(iswap), 60 Rz



72 sqrt(iswap), 108 Rz



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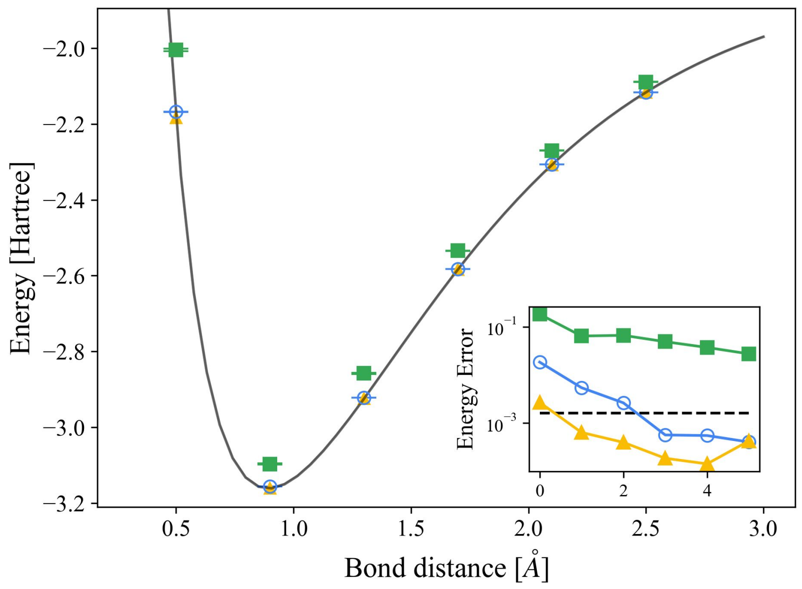

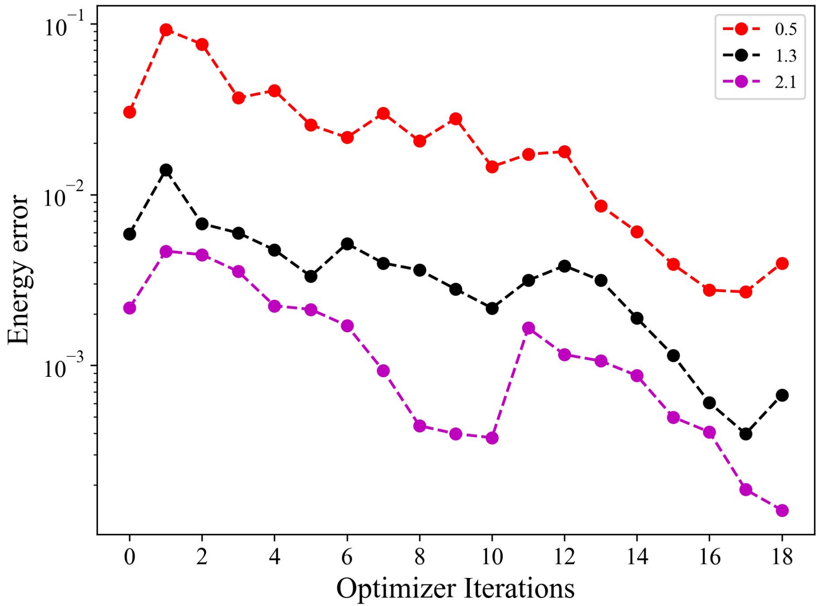

Used fact that gradient is function of 1-RDM

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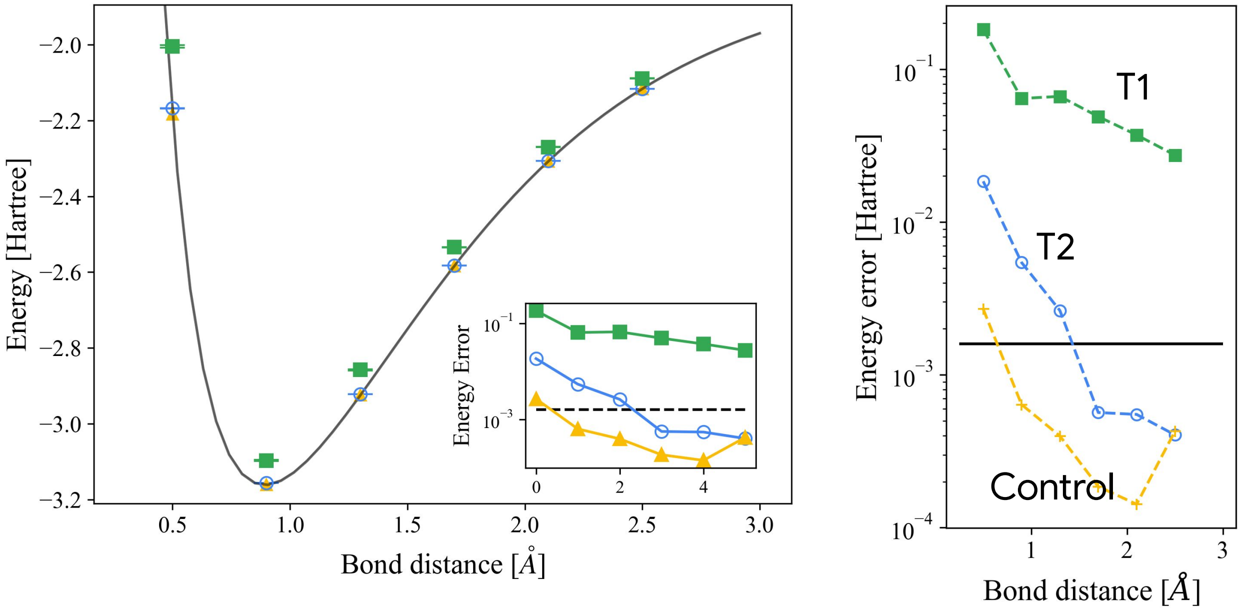
Hydrogen chain to benchmark out device



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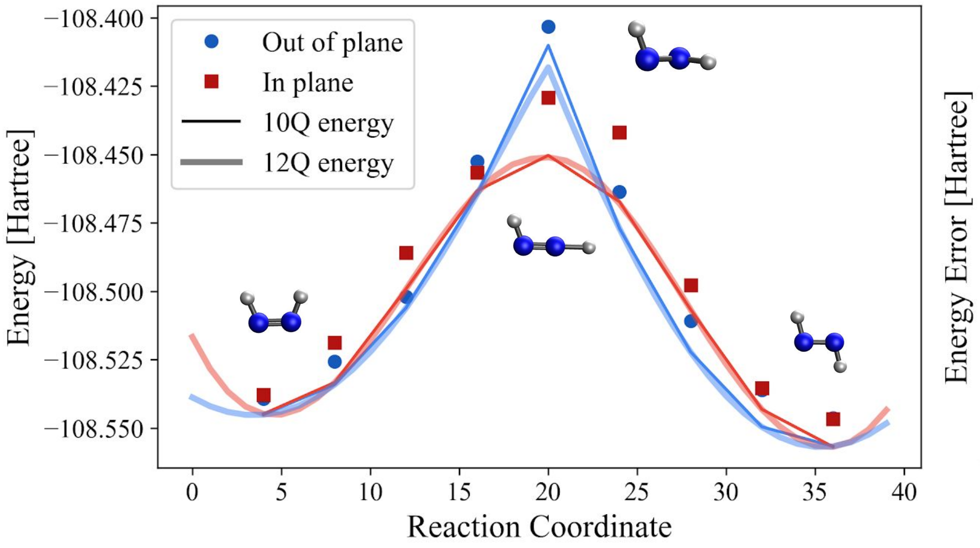
Starting to think about doing real chemistry

10 qubits, 0.050 [Hartree] separation between TS1 and TS2
Can we resolve this on Sycamore?



So what did we do / learn?

We realized the largest NISQ chemistry experiment <u>by far</u>
Good results up to 12 qubits but seems unlikely to scale past ~20 qubits with current error rates

Ansatz corresponded to arbitrary free fermion evolution (Hartree-Fock when optimized)
This is a classically tractable ansatz but still has a lot of entanglement and other nice properties

Algorithm performance improved a lot due to error-mitigation
Post-selection (T1), purification (T2), variational feedback (coherent errors)

Still, breakthrough might be required to scale to classically intractable regime
Or perhaps we "just" need error-correction!

Thank you!

Nick Rubin (led experiment)
Charles Neil (ran experiment)
Zhang Jiang (calibration / control)
Vadim Smelyanskiy (calibration / control)

Appendix Follows

Circuits for one-body rotations: Symmetries

Unrestricted spin [GHF]

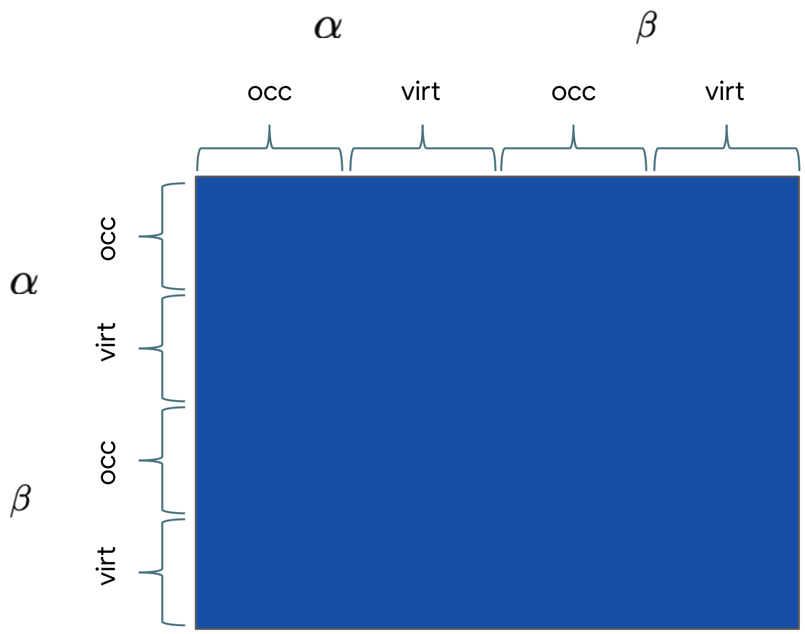
$$|\Phi\rangle = e^K a_1^\dagger e^{-K} \ldots e^K a_n^\dagger e^{-K} |0\rangle$$
$$= e^K a_1^\dagger \ldots a_n^\dagger |0\rangle$$

$$K = \sum_{pq} \kappa_{p,q} a_p^\dagger a_q$$
$$K = -K^\dagger$$

Restricted spin [UHF/RHF]

$$K_{\mathrm{UHF}} = \sum_{p>q} \kappa^{\alpha}_{p,q} \left(a^\dagger_{p\alpha} a_{q\alpha} - a^\dagger_{q\alpha} a_{p\alpha}\right) + \sum_{p>q} \kappa^{\beta}_{p,q} \left(a^\dagger_{p\beta} a_{q\beta} - a^\dagger_{q\beta} a_{p\beta}\right)$$

$$K_{\mathrm{RHF}} = \sum_{p>q} \kappa_{p,q} \left(a^\dagger_{p\alpha} a_{q\alpha} + a^\dagger_{p\beta} a_{q\beta} - a^\dagger_{q\alpha} a_{p\alpha} - a^\dagger_{q\beta} a_{p\beta}\right)$$



Circuits for one-body rotations: Symmetries

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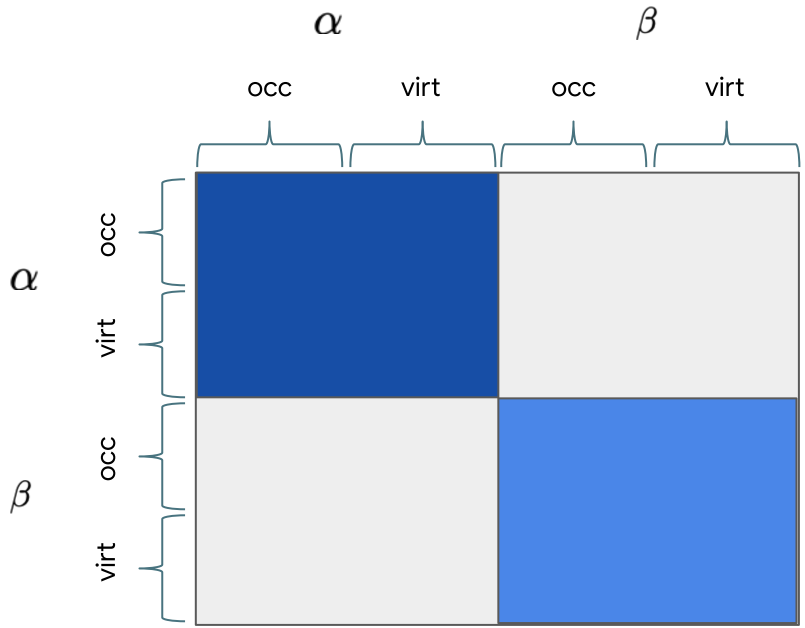

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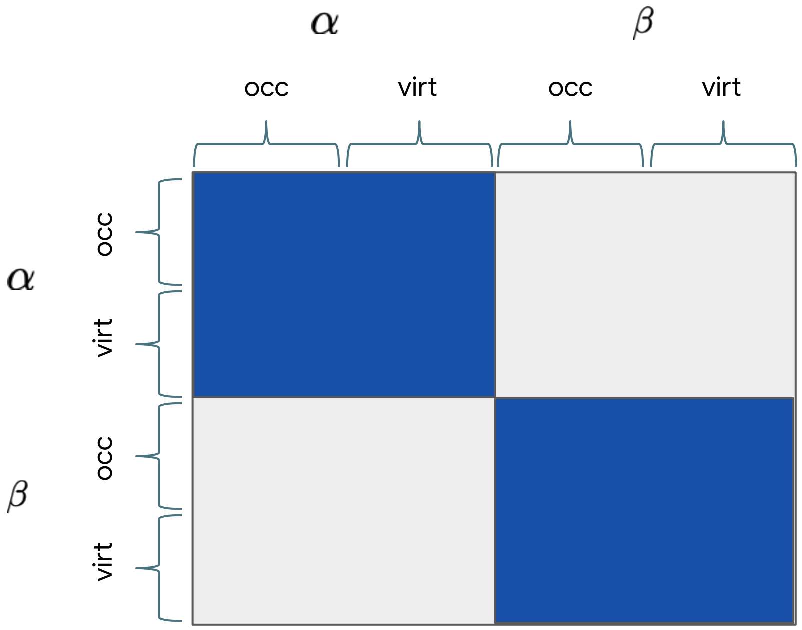

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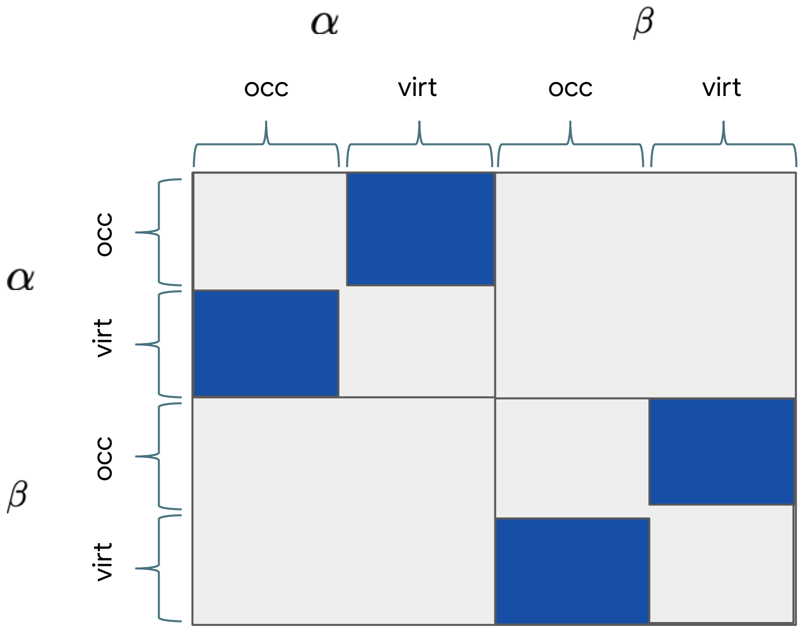

Additional restriction due to removal of redundant rotations

Measurements?

For product state energy can be evaluated by measuring all pairwise correlators

$$^2D^{pq}_{ij} = \langle \phi(\theta) | a^\dagger_p a^\dagger_q a_j a_i | \phi(\theta) \rangle = \frac{1}{2}\left({}^1D^p_i \, {}^1D^q_j - {}^1D^q_i \, {}^1D^p_j \right)$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} \langle \hat{a}^\dagger_i \hat{a}_j \rangle + \sum_{ijkl} V_{ijkl} \langle \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k \rangle$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} \, {}^1D^i_j + \sum_{ijkl} V_{ijkl} \, {}^2D^{ij}_{lk}$$

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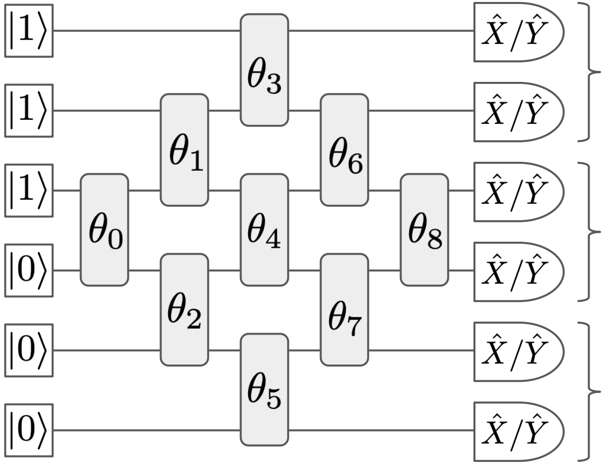
$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} {}^1D^i_j + \sum_{ijkl} V_{ijkl} {}^2D^{ij}_{lk}$$

Goal: measure the 1-RDM: $\langle \psi | a^\dagger_i a_j | \psi \rangle$



$$\langle a^\dagger_1 a_0 \rangle + \langle a^\dagger_0 a_1 \rangle$$

$$\langle a^\dagger_2 a_1 \rangle + \langle a^\dagger_1 a_2 \rangle$$

$$\langle a^\dagger_3 a_2 \rangle + \langle a^\dagger_2 a_3 \rangle$$

$$\langle a^\dagger_4 a_3 \rangle + \langle a^\dagger_3 a_4 \rangle$$

$$\langle a^\dagger_5 a_4 \rangle + \langle a^\dagger_4 a_5 \rangle$$

Measurements?

For product state energy can be evaluated by measuring all pairwise correlators

$$^2D^{pq}_{ij} = \langle \phi(\theta) | a_p^\dagger a_q^\dagger a_j a_i | \phi(\theta) \rangle = \frac{1}{2}\left({}^1D^p_i {}^1D^q_j - {}^1D^q_i {}^1D^p_j \right)$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} \langle \hat{a}_i^\dagger \hat{a}_j \rangle + \sum_{ijkl} V_{ijkl} \langle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \rangle$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} {}^1D^i_j + \sum_{ijkl} V_{ijkl} {}^2D^{ij}_{lk}$$

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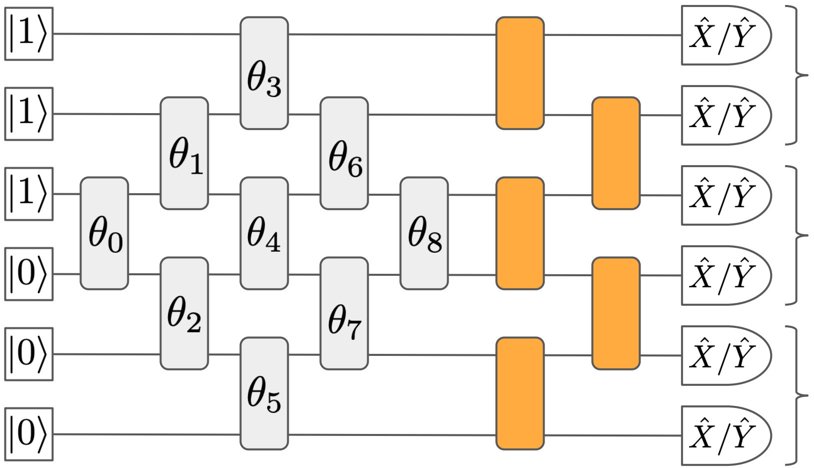

$$\langle a_3^\dagger a_1 \rangle + \langle a_1^\dagger a_3 \rangle$$
$$\langle a_0^\dagger a_3 \rangle + \langle a_3^\dagger a_0 \rangle$$
$$\langle a_5^\dagger a_0 \rangle + \langle a_0^\dagger a_5 \rangle$$
$$\langle a_2^\dagger a_5 \rangle + \langle a_5^\dagger a_2 \rangle$$
$$\langle a_4^\dagger a_2 \rangle + \langle a_2^\dagger a_4 \rangle$$

(orange gate) $= \exp(-i\pi \text{fswap}/2)$

$$\text{fswap} = a_p^\dagger a_q + a_q^\dagger a_p - a_p^\dagger a_p - a_q^\dagger a_q$$

Measurements?

For product state energy can be evaluated by measuring all pairwise correlators

$$ {}^2D^{pq}_{ij} = \langle\phi(\theta)|a_p^\dagger a_q^\dagger a_j a_i|\phi(\theta)\rangle = \frac{1}{2}\left({}^1D^{p}_{i}\,{}^1D^{q}_{j} - {}^1D^{q}_{i}\,{}^1D^{p}_{j}\right) $$

$$ \langle\hat{H}\rangle = \sum_{ij} h_{ij}\langle\hat{a}_i^\dagger\hat{a}_j\rangle + \sum_{ijkl} V_{ijkl}\langle\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_l\hat{a}_k\rangle $$

$$ \langle\hat{H}\rangle = \sum_{ij} h_{ij}\,{}^1D^{i}_{j} + \sum_{ijkl} V_{ijkl}\,{}^2D^{ij}_{lk} $$

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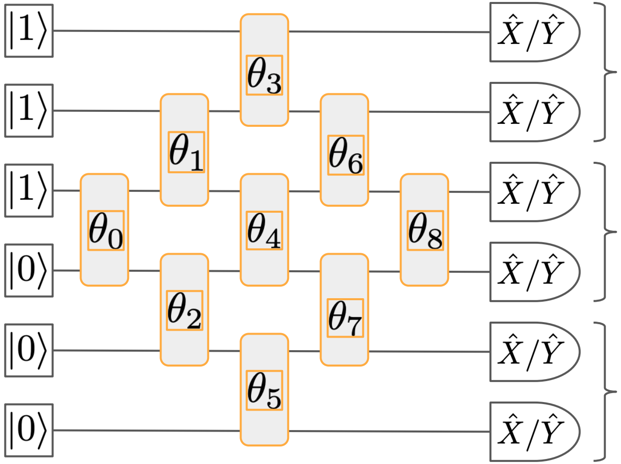
$$ U(u_a)\cdot U(u_b) = U(u_a\cdot u_b) $$



$$ \langle a_3^\dagger a_1\rangle + \langle a_1^\dagger a_3\rangle $$

$$ \langle a_0^\dagger a_3\rangle + \langle a_3^\dagger a_0\rangle $$

$$ \langle a_5^\dagger a_0\rangle + \langle a_0^\dagger a_5\rangle $$

$$ \langle a_2^\dagger a_5\rangle + \langle a_5^\dagger a_2\rangle $$

$$ \langle a_4^\dagger a_2\rangle + \langle a_2^\dagger a_4\rangle $$

Measurements?

For product state energy can be evaluated by measuring all pairwise correlators

$$^2D^{pq}_{ij} = \langle \phi(\theta) | a^\dagger_p a^\dagger_q a_j a_i | \phi(\theta) \rangle = \frac{1}{2} \left({}^1D^p_i \, {}^1D^q_j - {}^1D^q_i \, {}^1D^p_j \right)$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} \langle \hat{a}^\dagger_i \hat{a}_j \rangle + \sum_{ijkl} V_{ijkl} \langle \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k \rangle$$

$$\langle \hat{H} \rangle = \sum_{ij} h_{ij} \, {}^1D^i_j + \sum_{ijkl} V_{ijkl} \, {}^2D^{ij}_{lk}$$

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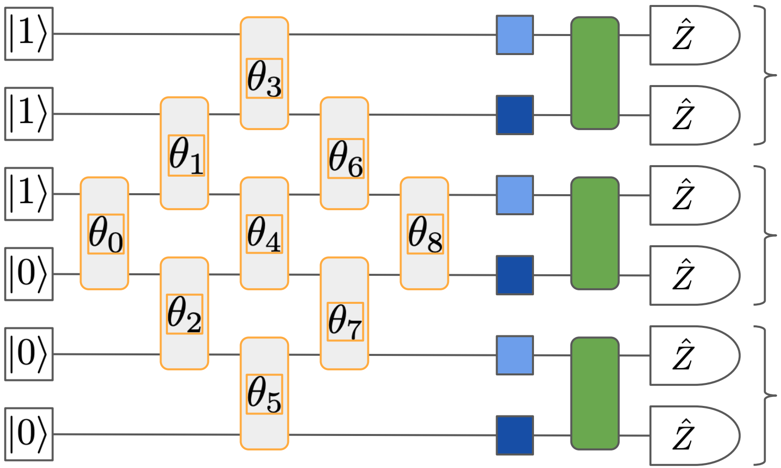
$$U(u_a) \cdot U(u_b) = U(u_a \cdot u_b)$$



$$\langle a^\dagger_3 a_1 \rangle + \langle a^\dagger_1 a_3 \rangle$$

$$\langle a^\dagger_0 a_3 \rangle + \langle a^\dagger_3 a_0 \rangle$$

$$\langle a^\dagger_5 a_0 \rangle + \langle a^\dagger_0 a_5 \rangle$$

$$\langle a^\dagger_2 a_5 \rangle + \langle a^\dagger_5 a_2 \rangle$$

$$\langle a^\dagger_4 a_2 \rangle + \langle a^\dagger_2 a_4 \rangle$$