Title: Unbiasing Fermionic Quantum Monte Carlo with a Quantum Computer

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Abstract: Many-electron problems pose some of the greatest challenges in computational science, with important applications across many fields of modern science. Fermionic quantum Monte Carlo (QMC) methods are among the most powerful approaches to these problems. However, they can be severely biased when controlling the fermionic sign problem using constraints, as is necessary for scalability. Here we propose an approach that combines constrained QMC with quantum computing tools to reduce such biases. We experimentally implement our scheme using up to 16 qubits in order to unbias constrained QMC calculations performed on chemical systems with as many as 120 orbitals. These experiments represent the largest chemistry simulations performed on quantum computers (more than doubling the size of prior electron correlation calculations), while obtaining accuracy competitive with state-of-the-art classical methods. Our results demonstrate a new paradigm of hybrid quantum-classical algorithm, surpassing the popular variational quantum eigensolver in terms of potential towards the first practical quantum advantage in ground state many-electron calculations.

Quantum AI

Unbiasing Fermionic Quantum Monte Carlo with a Quantum Computer

William J. Huggins, Perimeter Institute, Feb 2022

Google

Gratitude

Co-authors

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Google collaborators

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Projector Monte Carlo

Quantum AI

The electronic structure problem

We have a Hamiltonian

$$H(\mathbf{R}) = \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{pq} T(\mathbf{R})_{pq} a^\dagger_{p,\sigma} a_{q,\sigma} + \frac{1}{2} \sum_{\alpha,\beta \in \{\uparrow,\downarrow\}} \sum_{pqrs} V(\mathbf{R})_{pqrs} a^\dagger_{p,\alpha} a_{q,\alpha} a^\dagger_{r,\beta} a_{s,\beta}$$

The Hamiltonian encodes the physics

The $T(\mathbf{R})_{pq}$ terms and the $V(\mathbf{R})_{pqrs}$ terms together specify the problem, with space already discretized.

The ground state problem

Often the ground state is the only one with signficant occupation at room temperature.

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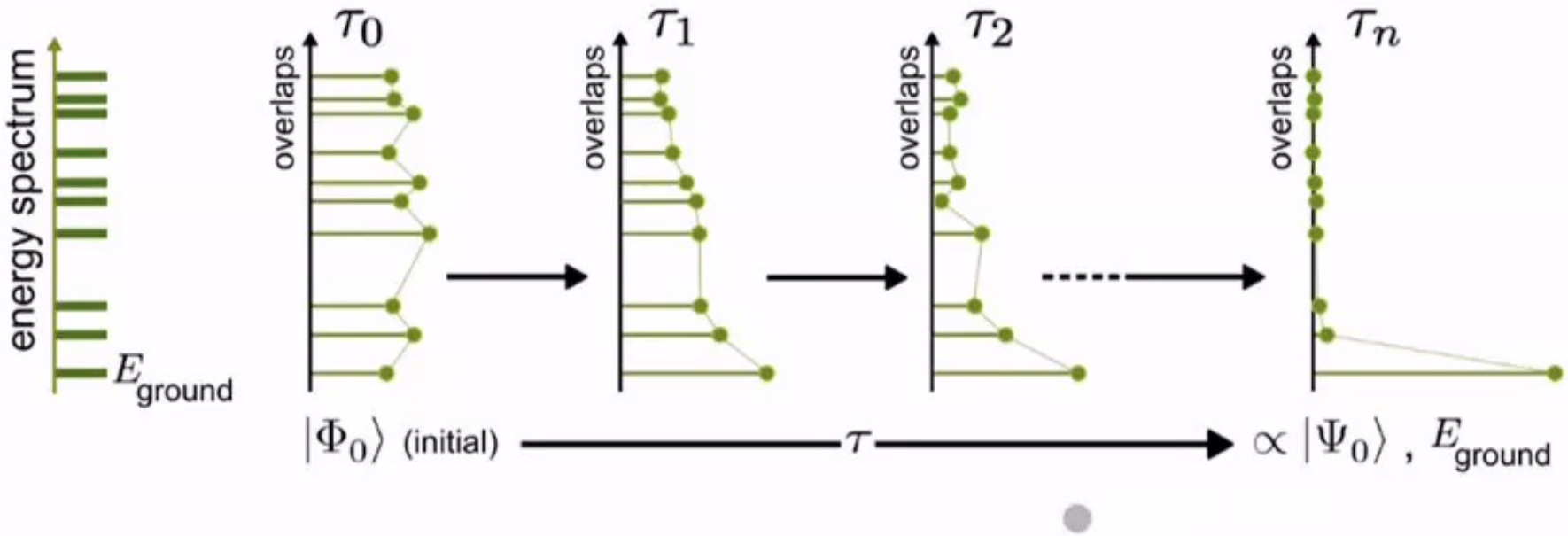
Imaginary time evolution

Project to the ground state

For any $|\psi_{\text{initial}}\rangle$ with non-zero overlap with the ground state,

$$\lim_{t\to\infty} e^{-tH} |\psi_{\text{initial}}\rangle \propto |\psi_{\text{ground}}\rangle .$$

Imaginary time evolution



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Projector Monte Carlo

Walkers

We represent represent $|\psi(\tau)\rangle$ as an ensemble of simple "walkers",

$$|\psi(\tau)\rangle = \sum_i w_i(\tau)\,|\phi_i(\tau)\rangle\,.$$

Propagator

We update the walkers using an approximation to the imaginary time propagator,

$$|\psi(\tau)\rangle \to |\psi(\tau+\Delta\tau)\rangle \approx e^{-\Delta\tau H}\,|\psi(\tau)\rangle\,.$$

Projector Monte Carlo

Many different realizations

Diffusion Monte Carlo, Green's Function Monte Carlo, Full Configuration Interaction Quantum Monte Carlo, **Auxiliary Field Quantum Monte Carlo (AFQMC)**...

Sometimes they work well

Bose-Einstein condensation of Helium 4 into a superfluid, unfrustrated bosons, Hubbard model at half-filling

Sometimes they struggle

Bose-Einstein condensation of Helium 3 into a superfluid, quantum chemistry, Hubbard model away from half-filling, most systems with fermions

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The (fermion) sign problem

- Collapse to the bosonic solution
- Catastrophic cancellation of contributions with different signs/phases

Auxiliary field quantum Monte Carlo

Walkers

In AFQMC, the walkers are Slater determinants.

Propagator

We use an approximation to the imaginary time evolution operator that maps Slater determinants to Slater determinants.

Auxiliary field quantum Monte Carlo

Rewrite the Hamiltonian

$$H = \sum_{pq} t_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q a_r^\dagger a_s \to \sum_{pq} t_{pq} a_p^\dagger a_q - \frac{1}{2} \sum_{\ell=1}^{L} v_\ell^2.$$

Trotter expansion

We take a Trotter expansion of $e^{-\Delta H}$.

The Hubbard-Stratonovich transformation

$$e^{\frac{\Delta}{2} v_\ell^2} \to \frac{1}{\sqrt{2\pi}} \int e^{\frac{-x^2}{2}} e^{\sqrt{\Delta} x v_\ell} dx$$

The sign problem in AFQMC is a phase problem

Multiple solutions

Imaginary time evolution converges to the ground state up to an arbitrary phase,

$$e^{iw} |\psi_{\text{ground}}\rangle .$$

The phase problem

Our ensemble average corresponds to a linear combination of these solution. The phases distribute uniformly over time.

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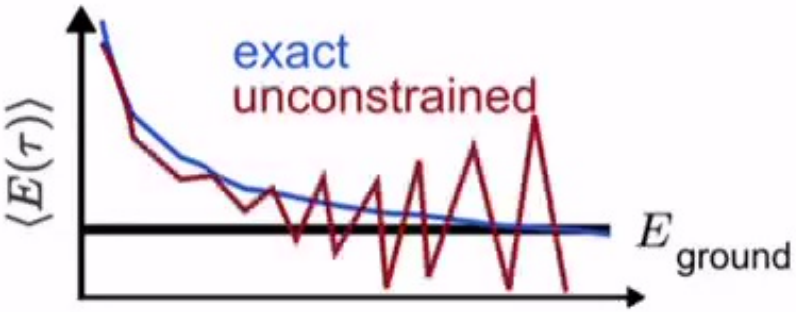

The phase problem

Our ensemble average corresponds to a linear combination of these solution. The phases distribute uniformly over time.

The phaseless approximation

Trial wavefunction

$$|\psi_{\text{trial}}\rangle \approx |\psi_{\text{ground}}\rangle$$

Biasing the random walk

With a trial wavefunction we can bias the random walk and break the symmetry.

We force the overlap between the walker and the trial wavefunction to be positive,

- $\langle \phi_i(\tau) | \psi_{\text{trial}} \rangle \in \mathbb{R}^+$.

The phaseless approximation

Impact of the trial wavefunction

AFQMC energies are usually much better than the bare trial wavefunction energies.

AFQMC is exact in the limit where the trial wavefunction is exact.

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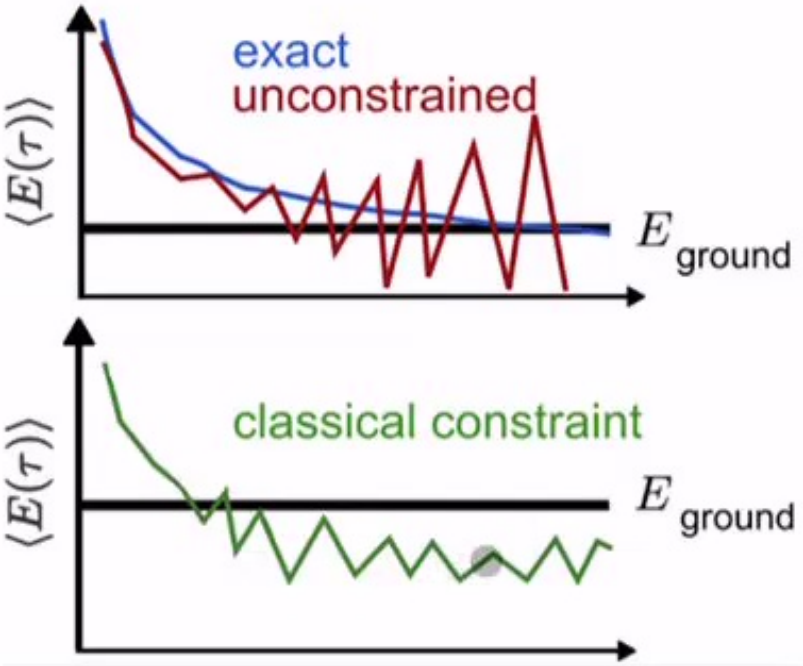

Quantum trial wavefunctions

With a quantum computer, we can efficiently approximate the overlap for a much wider range of trial wavefunctions.

- Unitary Coupled Cluster
- Tensor Networks
- Adiabatic State Preparation
- Hardware Efficient Ansatz
- ...

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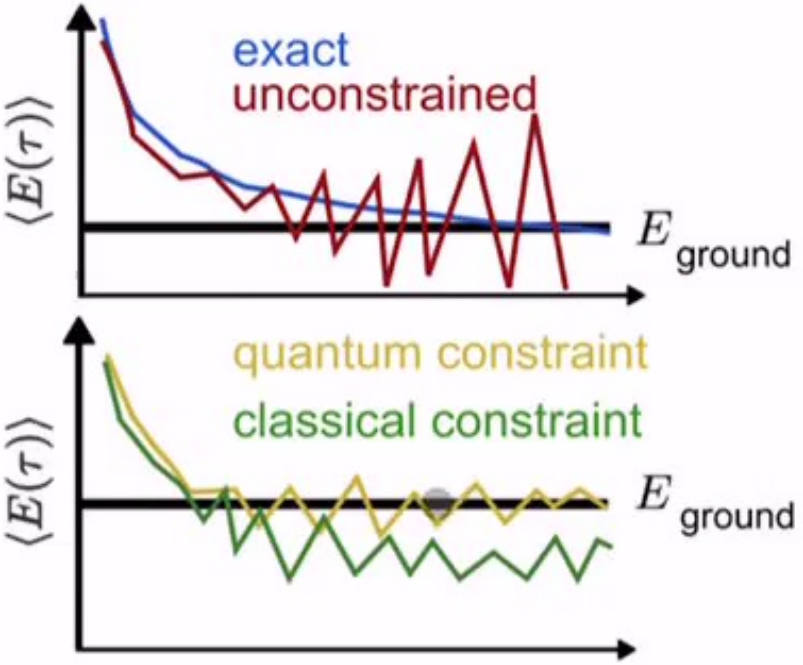

Shadow Tomography

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Shadow tomography[1]

- Take a copy of your input state ρ
- Apply a randomly chosen circuit U_i from an ensemble $\mathcal{U}$ (Clifford circuits here)

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- Take a copy of your input state ρ
- Apply a randomly chosen circuit U_i from an ensemble $\mathcal{U}$ (Clifford circuits here)
- Measure in the computational basis to obtain the bitstring b_i
- Rinse and repeat, saving a record of the U_is and b_is (the classical shadow)

[1] Huang, H.-Y., Kueng, R. & Preskill, J. Predicting many properties of a quantum system from very few measurements. Nat. Phys. 16, 1050–1057 (2020).

Shadow tomography

Measurement as an invertible quantum channel

Shadow tomography with Clifford circuits defines an invertible quantum channel $\mathcal{M}$,

$$\mathcal{M}(\rho) := \mathbb{E}_{U\sim \mathrm{Cl}(2^N)} \sum_{b\in\{0,1\}^N} \langle b|U\rho U^\dagger|b\rangle\, U^\dagger\,|b\rangle\langle b|\, U.$$

The inverse has a simple closed form,

$$\mathcal{M}^{-1}(A) = (2^N-1)A - \mathbb{I}.$$

The classical shadow of ρ is an approximate reconstruction of ρ obtained by sampling,

$$\rho = \mathbb{E}_{U\sim \mathrm{Cl}(2^N)} \sum_{b\in\{0,1\}^N} \langle b|U\rho U^\dagger|b\rangle\, \mathcal{M}^{-1}\left(U^\dagger\,|b\rangle\langle b|\, U\right).$$

Shadow tomography

Shadow norm

The number of samples we require to estimate M different observables, each to within a precision ϵ, scales as

$$\log(M)\max_i ||O_i||_{\text{shadow}}/\epsilon^2.$$

For the Clifford group on N qubits,

$$||O_i||_{\text{shadow}} \leq 3\,\text{tr}\left(O^2\right)$$

Scaling

We only need to perform $O(log(M)\epsilon^{-2})$ measurements to estimate the overlap of the trial wavefunction with M different Slater determinants, each to within a precision ϵ.

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The protocol

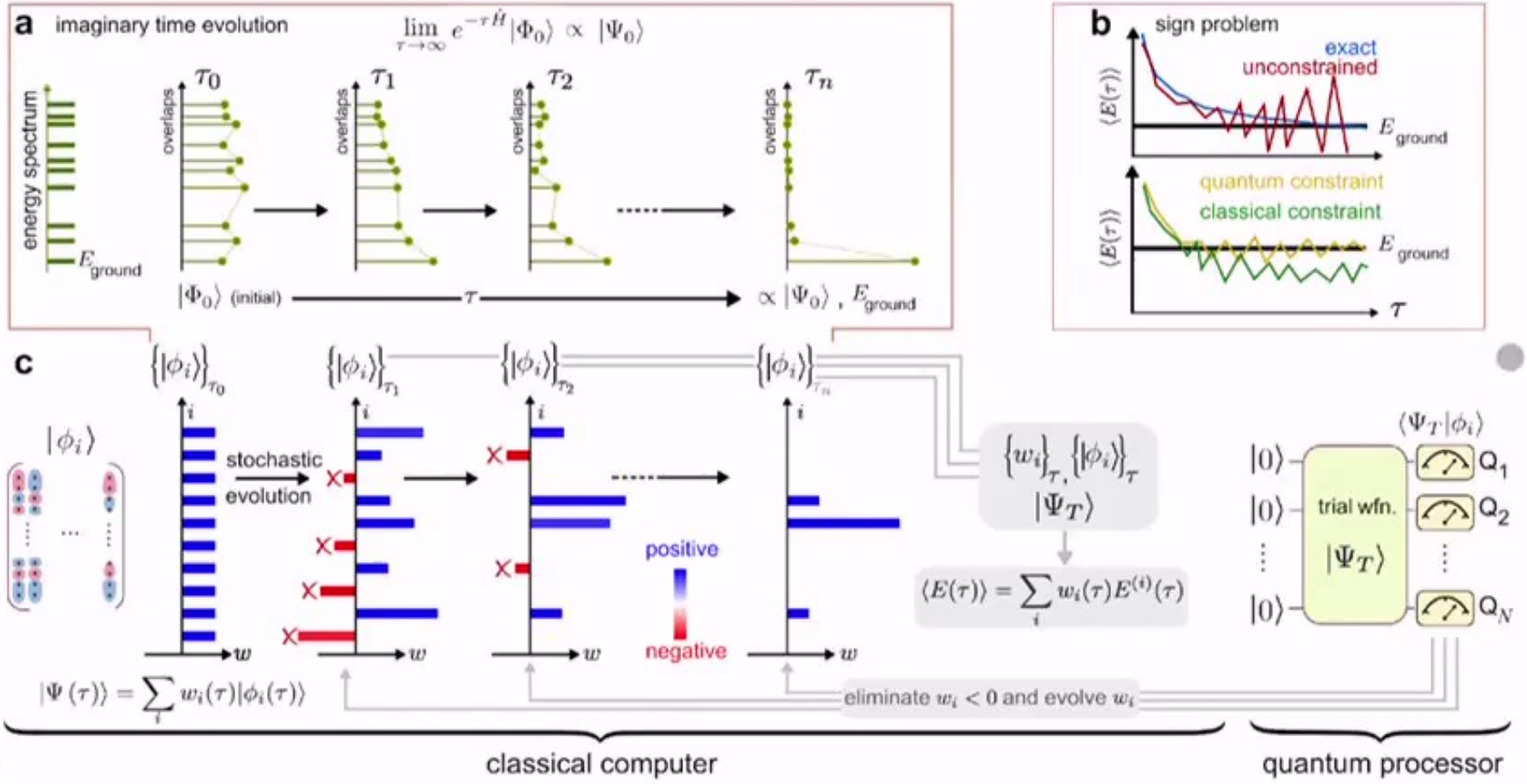
Collect the classical shadow

- Characterize the state $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|\psi_{\text{trial}}\rangle$
- We can approximate $\langle\phi|\psi_{\text{trial}}\rangle$ using expectation values of $P_+ = |\phi\rangle\langle\psi_{\text{trial}}| + |\psi_{\text{trial}}\rangle\langle\phi|$ and $P_- = i|\phi\rangle\langle\psi_{\text{trial}}| - i|\psi_{\text{trial}}\rangle\langle\phi|$

Offline AFQMC calculation

- Nearly standard AFQMC calculation
- All quantities expressed in terms of wavefunction overlaps

The protocol



Reasons for hope

Modest measurement cost

No feedback loop between classical and quantum processors

Biasing a random walk

Inherent noise resilience

Eight qubit experiment

The system

We consider a toy version of a hard problem, a square arrangement of four Hydrogen atoms. We consider both an STO-3G basis set (4 orbitals / 8 qubits) **and a cc-pVQZ basis set (120 orbitals / 240 qubits)**.

The ansatz

We start with a well-studied ansatz known as Perfect Pairing:

$$|\Psi_{\mathrm{PP}}\rangle = e^{\hat{T}_{\mathrm{PP}}} |\psi_0\rangle\,, \qquad \hat{T}_{\mathrm{PP}} = \sum_{i}^{N_{\mathrm{pairs}}} t_i \hat{a}^{\dagger}_{i^*_\uparrow} \hat{a}_{i_\uparrow} \hat{a}^{\dagger}_{i^*_\downarrow} \hat{a}_{i_\downarrow}\,.$$

Then we add several layers of hardware-efficient gates and an offline orbital rotation.

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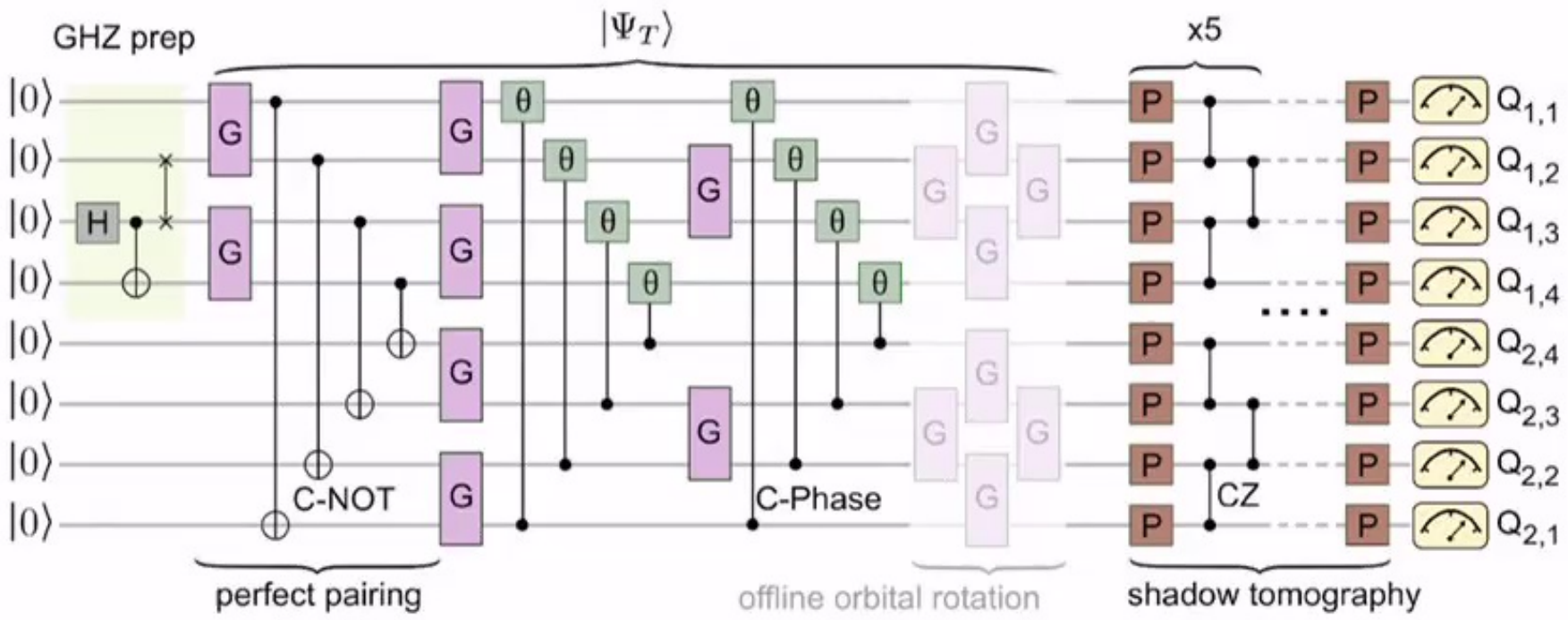
Eight qubit experiment



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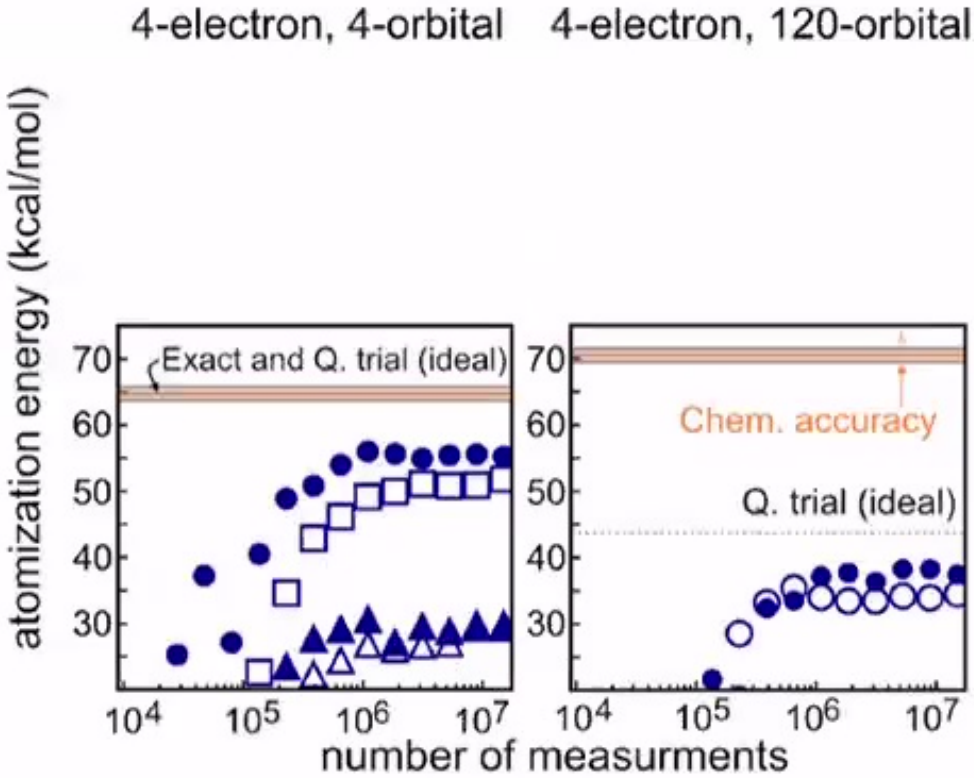
Eight qubit experiment

Observations

- The energy on the left would be exact without noise.
- All experiments are far from chemical accuracy (pale orange band).



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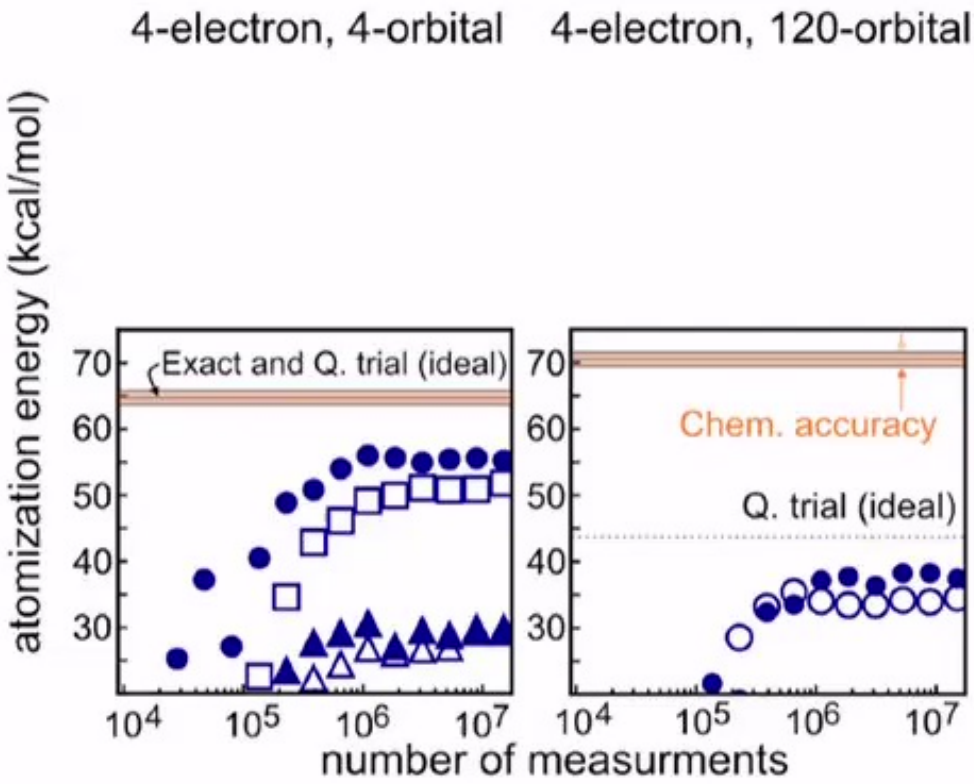
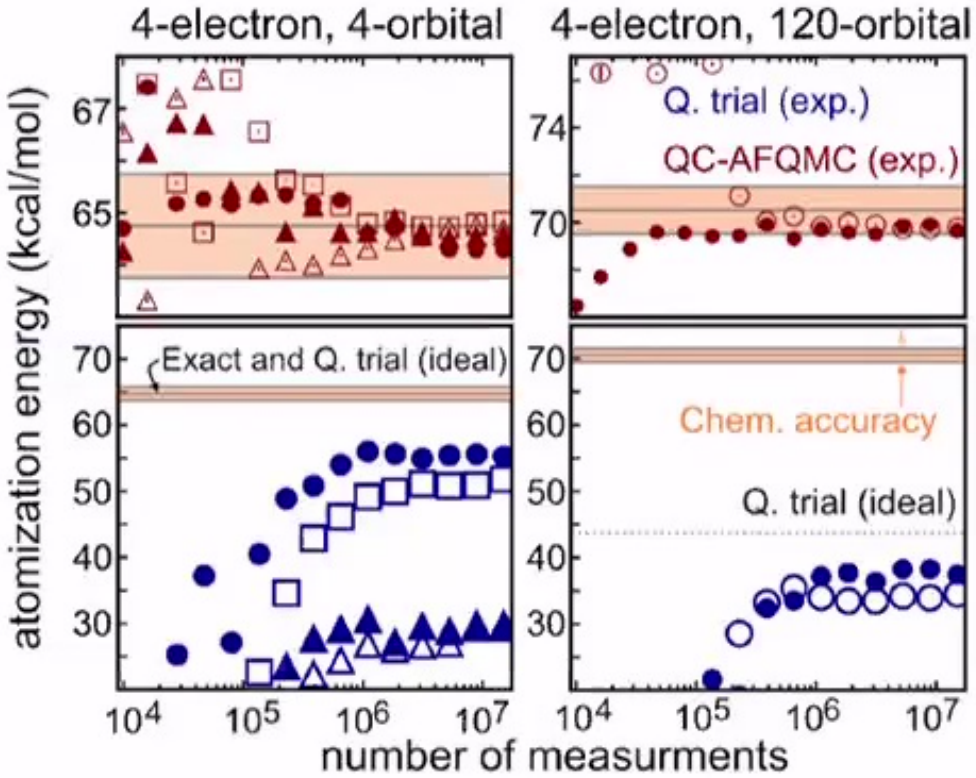


Quantum AI

Eight qubit experiment

Observations

- The energy on the left would be exact without noise.
- All experiments are far from chemical accuracy (pale orange band).
- QC-AFQMC energies are all within chemical accuracy.
- QC-AFQMC suppresses the variation between experiments.



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Twelve and sixteen qubit experiments

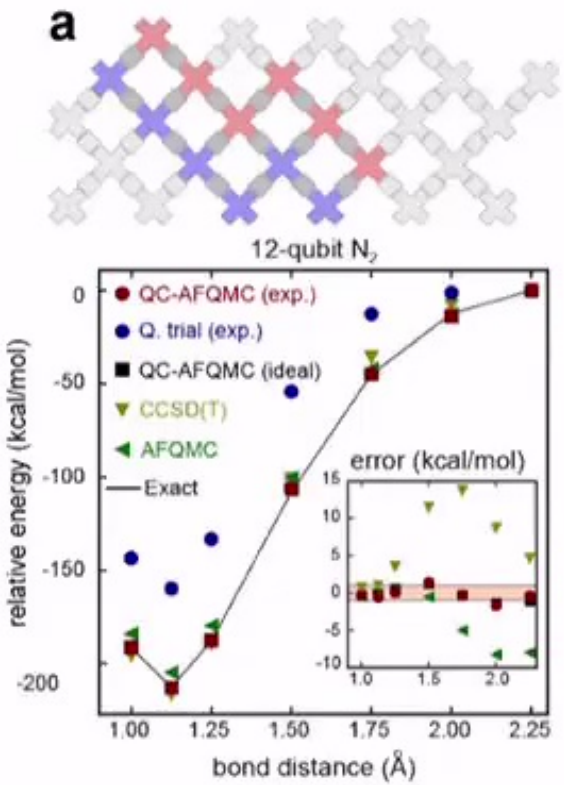
Twelve qubits

- Nitrogen dimer potential energy surface
- cc-PVTZ basis (60 orbitals)
- Perfect pairing ansatz

Sixteen qubits

- Diamond crystal
- Two atom unit cell
- Finite size effects
- DZVP-GTH basis (26 orbitals)
- Perfect pairing ansatz

Twelve qubit experiment



Observations

- The experimental QC-AFQMC energies (blue circles) are close to the noiseless QC-AFQMC energies (black squares).
- QC-AFQMC produces energies competetive with other state-of-the-art approaches.

Quantum AI

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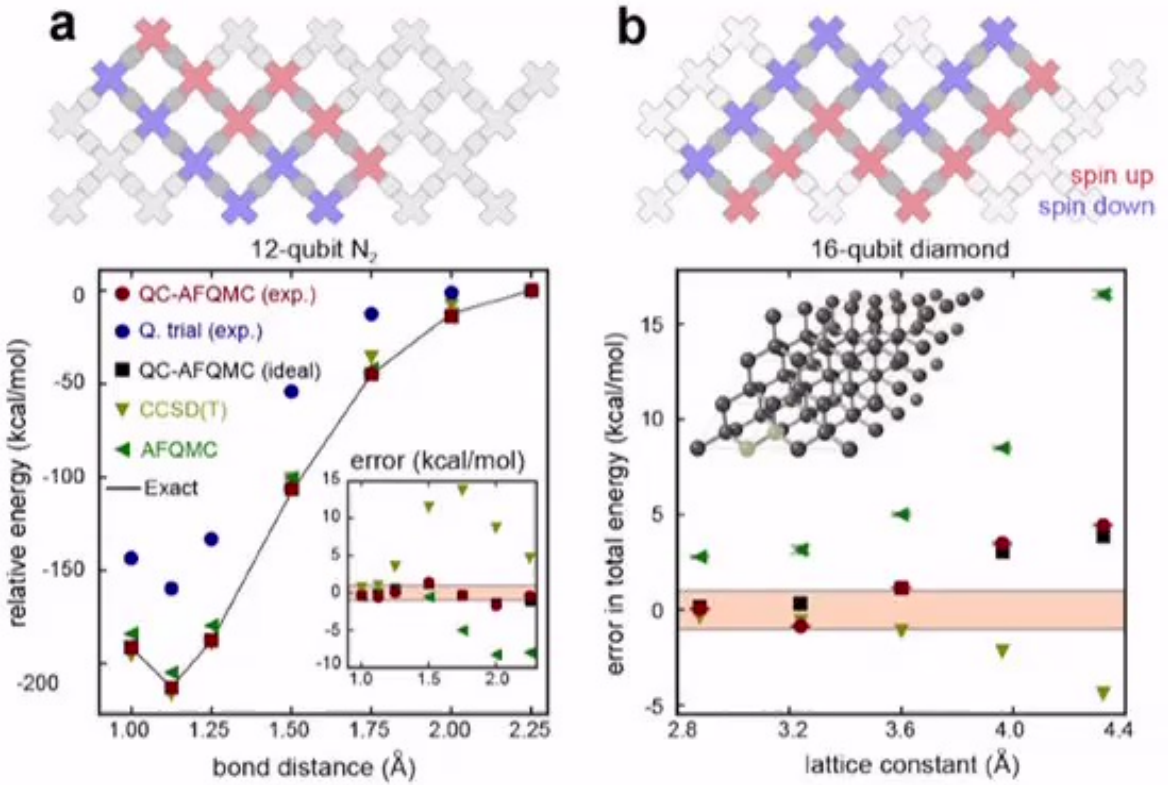

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Thank You

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