Unbiasing Fermionic Quantum Monte Carlo with a Quantum Computer

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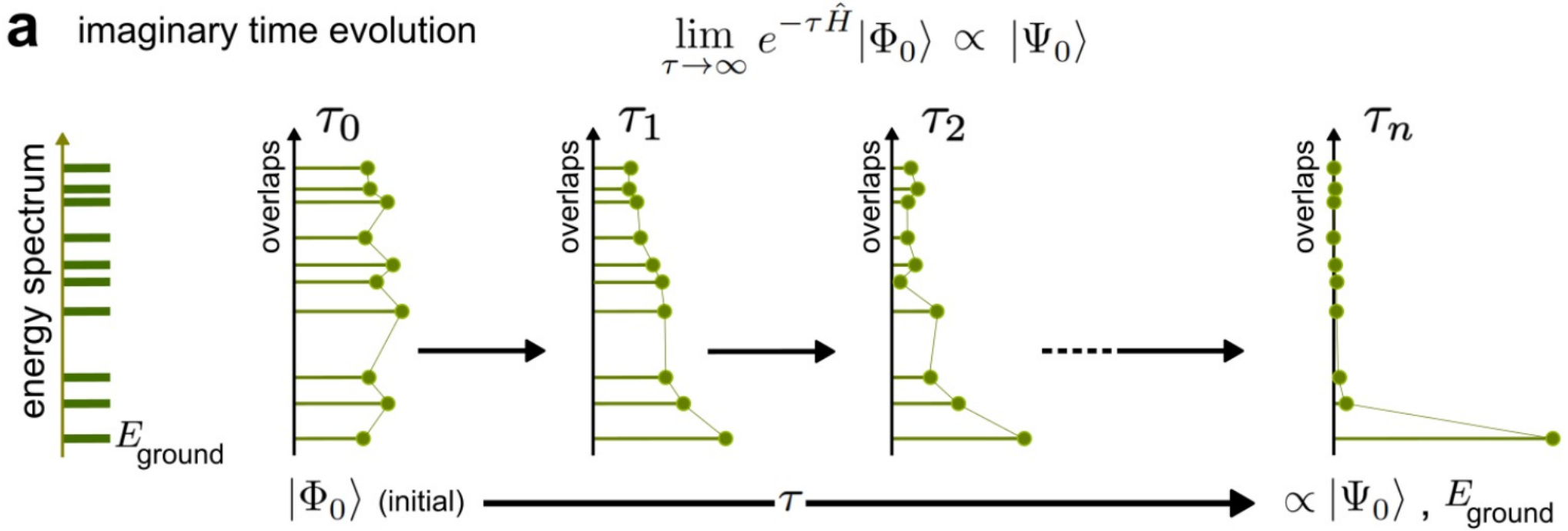
- As imaginary time progresses, the energy of the current wavefunction should tend towards the ground state energy of H.

Imaginary Time Evolution



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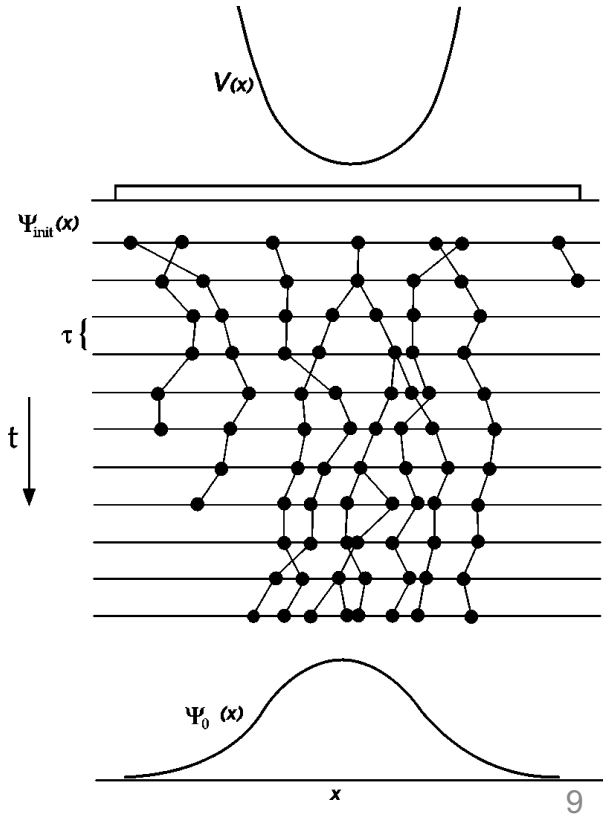

https://www.researchgate.net/figure/Illustration-of-the-walker-evolution-in-the-diffusion-Monte-Carlo-DMC-method-The_fig1_2464596

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- We must map the quantum partition function to the classic analogue:

$$Z = Tr[e^{-\beta H}] \rightarrow \sum_i e^{-\beta E_i}$$

- Inside the summation, these are the Boltzmann weights, $w(i) = e^{-\beta E_i}$, (which classically are positive or zero)

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- Combinations of positive and negative Boltzmann weights yield exponential growth in the statistical errors (proof is omitted for brevity)

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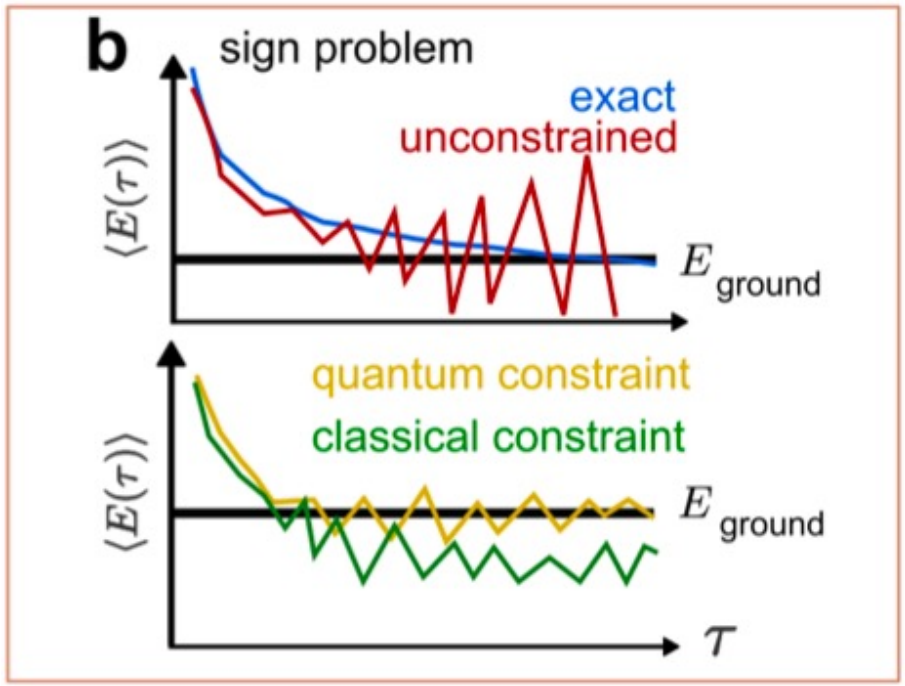

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- In this paper, the "fixed node" approximation is one constraint used (delete any negative weights)

Quantum-Classical Hybrid AFQMC Algorithm (QC-AFQMC)

- The energy in AFQMC is given by $E(\tau) = \frac{\langle \Psi_T | \hat{H} | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle}$
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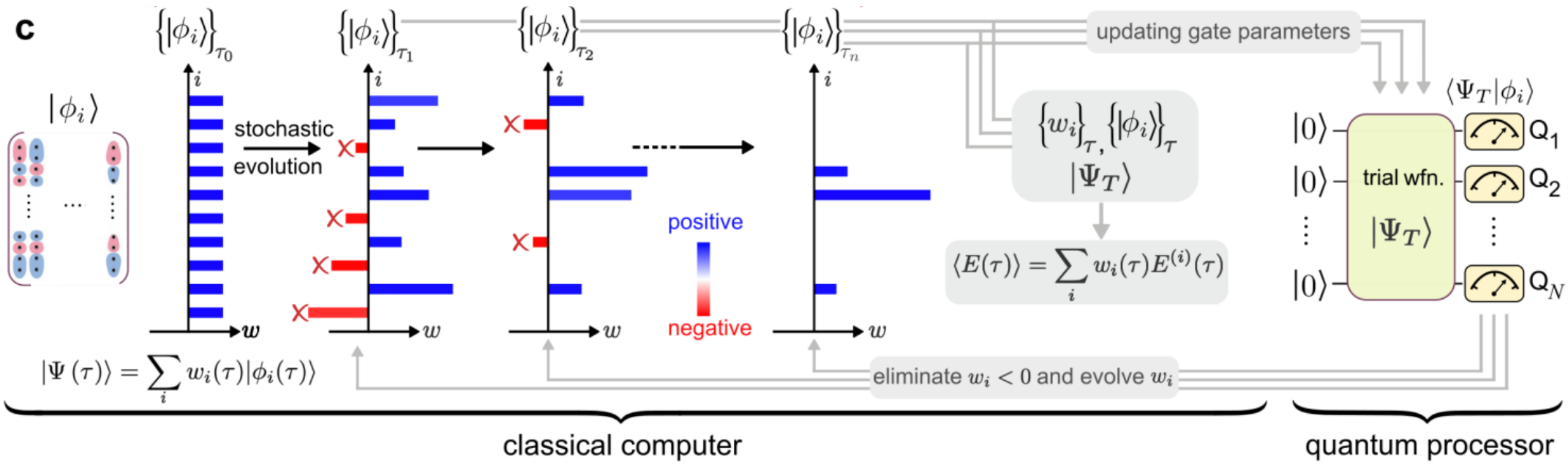
- We need to calculate $\langle \Phi_T | \phi_i(\tau) \rangle$ for each walker and every timestep
- This is inefficient on a classical computer, but efficient on a quantum computer
- How can we utilize both the classical and quantum processors to maximize the efficiency?

QC-AFQMC Overview



Results

- Experiments were performed using Google's 54 qubit processor *Sycamore*
- We are interested in the atomization energy of the following molecules:
  - H_4
  - N_2
  - Diamond

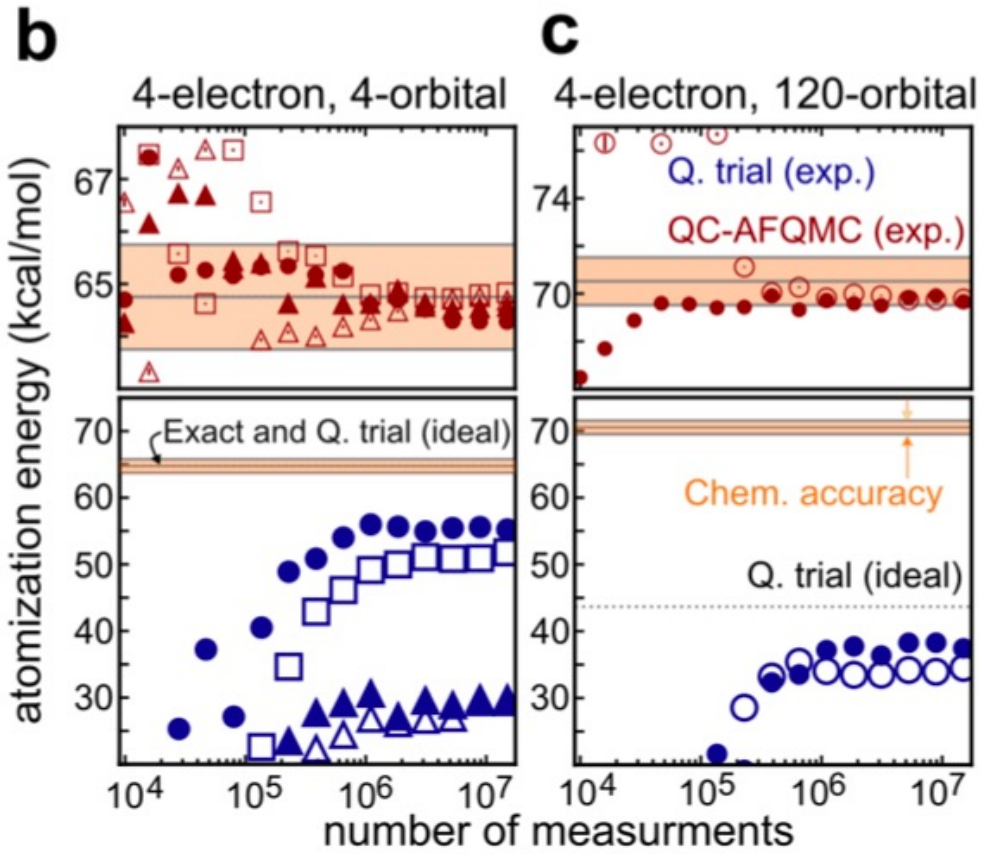
H_4

- We start with a square geometry

	Exact	AFQMC	QC-AFQMC
4 Orbital	64.7	62.9	64.3
120 Orbital	70.5	68.6	69.7

Atomization Energy of H_4 (kcal/mol)

H_4

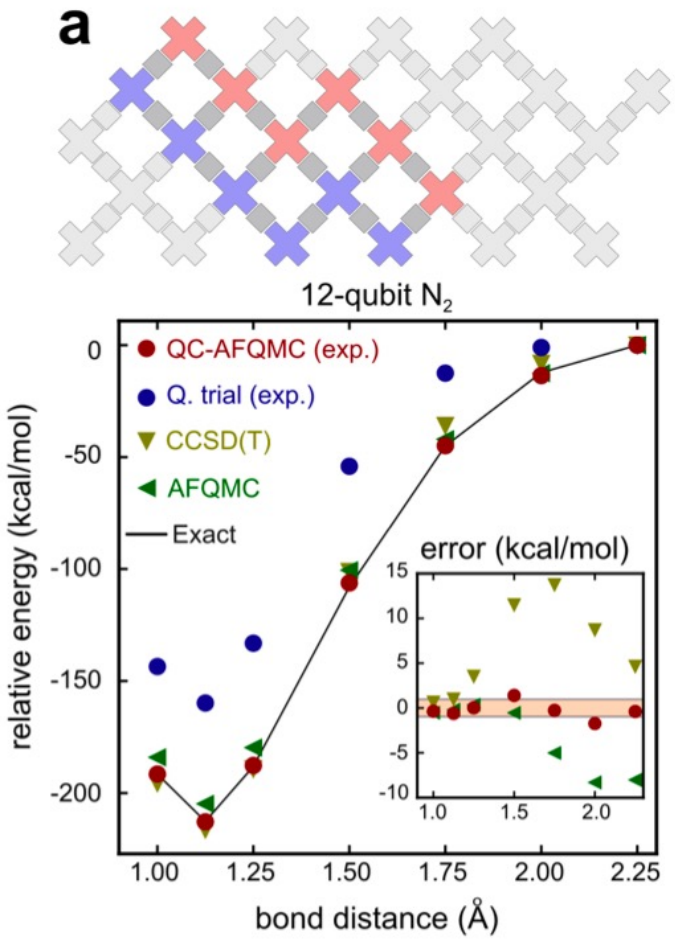


- Each style of dot represents a different run
- For both basis sets, QC-AFQMC converges on the order of 10^7 measurements
- For the 120-orbital basis set, QC-AFQMC converges even quicker

N_2

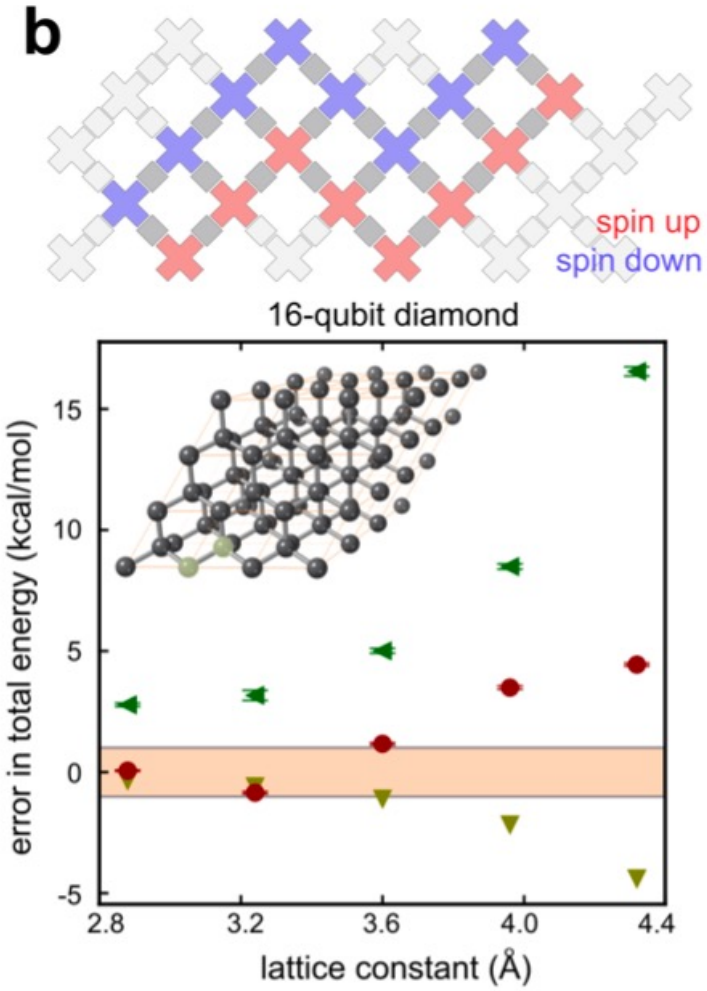
- In this experience, 12 qubits are used
- We use a linear geometry:

- Again, QC-AFQMC gives closest results (however, not within chem. Accuracy 1kcal/mol)
- Takeaway: Even with a simple trial wavefunction, our energies are close to those from state-of-the-art tech.



Diamond

- In this experiment, the lattice constant of diamond is being discovered with 16 qubits
- At this size, the model exhibits significant finite-size effects
- Correct experimental lattice constant not predicted
- This is the largest-to-date simulation quantum computer (as of July 2021)
- QC-AFQMC is as accurate as state-of-the-art method for a range of lattice constants



Source

- “Unbiasing Fermionic Monte Carlo with a Quantum Computer”
  - https://arxiv.org/pdf/2106.16235.pdf