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Hamiltonian simulation

Benchmarked on a trapped-ion quantum computer

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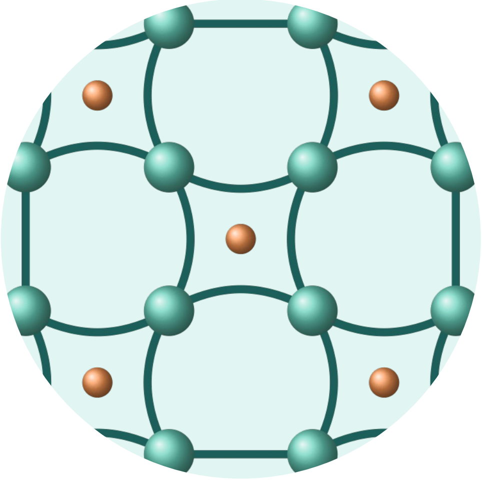
Applications of Hamiltonian simulation

One of the simplest tasks that quantum computers can perform exponentially faster



Simulating quantum physical systems

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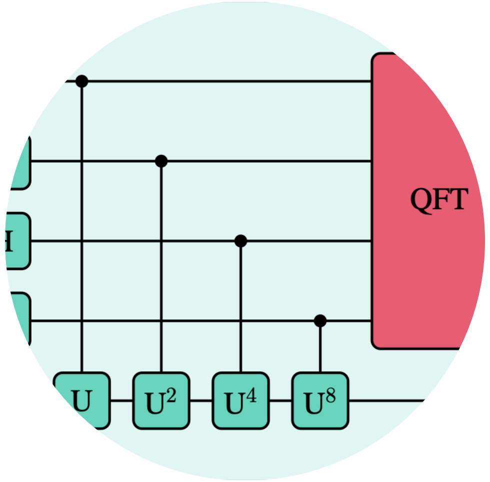
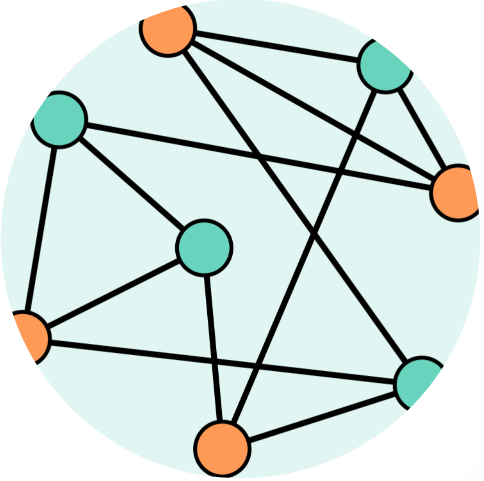
original motivation for quantum computers



Sub-routine to algorithms, such as Quantum Phase Estimation

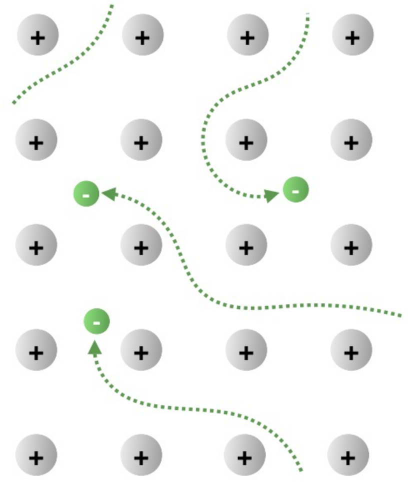


Adiabatic algorithm for classical optimization

Application-oriented benchmark use case

Example of application: the Hubbard model

- Need for quantum computer benchmarks that are **as close to applications as possible**.
- Simulating materials often means simulating **fermionic systems** (electrons).
- Natural near-term goal/benchmark for Hamiltonian simulation on quantum computers: the **Hubbard model** for high-temperature superconductivity



$$H = \quad -J \sum_{\langle i,j \rangle, \sigma} c^{+}_{i,\sigma} c_{j,\sigma} + c^{+}_{j,\sigma} c_{i,\sigma} \quad + \quad U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

with $c^{+}_{j,\uparrow}$ fermionic creation operators,
and $n_{j,\sigma} = c^{+}_{j,\sigma} c_{j,\sigma}$ the density of fermions.

Some figures:

- More than 50,000 papers written in 60 years.
- In the USA, around $20M/year is spent for simulation of this model

[Agrawal et al, 2406.06511]

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Benchmarking Hamiltonian simulation

How to benchmark the quality of a quantum computer implementation?

- No possible direct evaluation of Hamiltonian simulation, contrary to other applications. Need for comparison data.
- Scalability? Current hardware is at the frontier of classically simulable regime. [Haghshenas et al, arXiv:2503.20870]

Informative but not scalable:

- **State-vector simulation**: exponential in number of qubits
- **Tensor network simulations:** exponential in simulation time

Scalable but less informative:

- **Mirror circuits**: systematically over-estimate noise in Hamiltonian simulation [Granet Dreyer, PRX Quantum 6, (2025)]
- **Conserved quantities** (like particle number): very sensitive to certain errors, and insensitive to others
- **Clifford circuits**: too dissimilar to actual circuits (large gate angles)

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A scalable benchmark

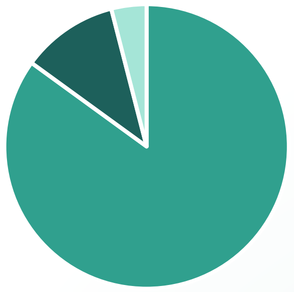
Non-interacting fermions

- Implementing the **kinetic part** of the Hamiltonian is $\mathbf{85\%}$ of our total two-qubit gate cost.

- With just the kinetic term, the circuit is classically simulable in **polynomial time**.

$$H = \quad -J \sum_{\langle i,j\rangle,\sigma} c^{+}_{i,\sigma} c_{j,\sigma} + c^{+}_{j,\sigma} c_{i,\sigma} \quad + \quad U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

Two-qubit gates in one Trotter step



- Relatively small modification of the circuit that allows for **scalable and informative benchmark**.

Benchmark protocol

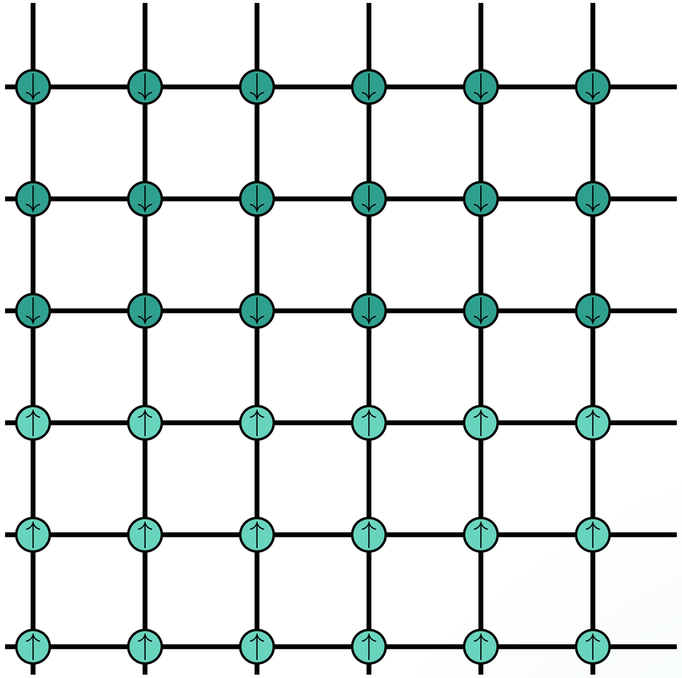
Definition

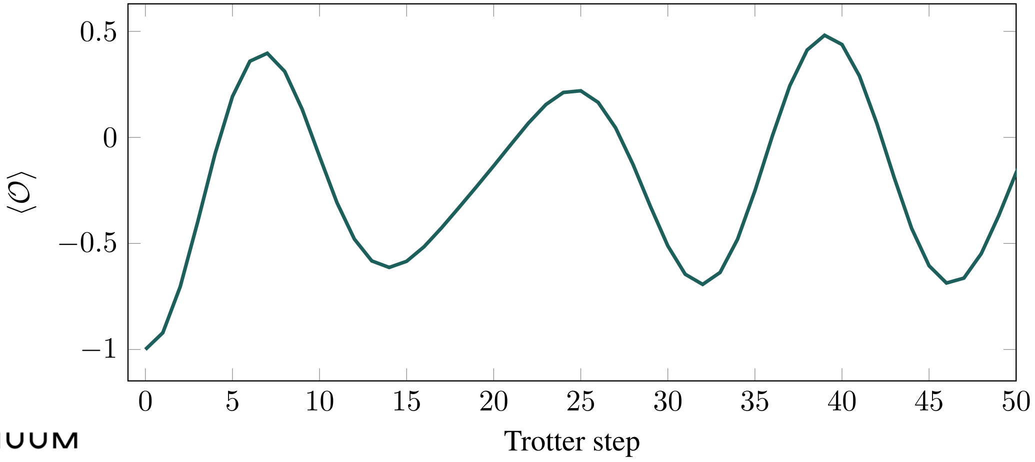
Single benchmark parameter: linear system size L.

- $L \times L$ square lattice. Hilbert space dimension 2^{2L^2}
- Initialize one fermion on each site, up (down) spins in the lower (upper) half.
- Time evolution with a **Trotter** product formula.
- Measure the imbalance of down/up spins

$$\mathcal{O} = \frac{2}{L^2} \sum_{upper\ half} n_{j,\uparrow} - n_{j,\downarrow}$$

at $2L$ times $dt, 2dt, 3dt, \ldots$ with $dt = 0.2$.





- architecture-agnostic geometry
- slow evolution, on a time scale $O(L)$
- low variance over shots

Compact encoding

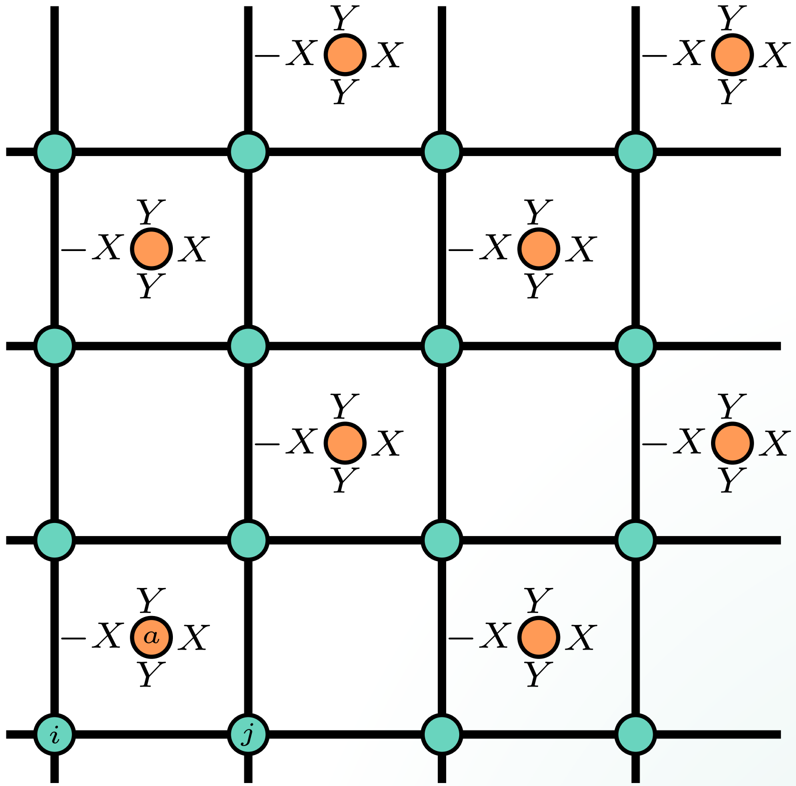
Implementing fermionic statistics with qubits

- Fermions **anticommute**, $c_i c_j = -c_j c_i$. This has to be **encoded** with qubits.

- We use the **compact encoding**. It implements the anticommutation through ancillas

$$c_i^{+} c_j + c_j^{+} c_i = \frac{1}{2}(X_i P_a X_j + Y_i P_a Y_j)$$

- Requires $L^2/2$ ancillas initially prepared in the ground state of the **toric code** on the lattice.

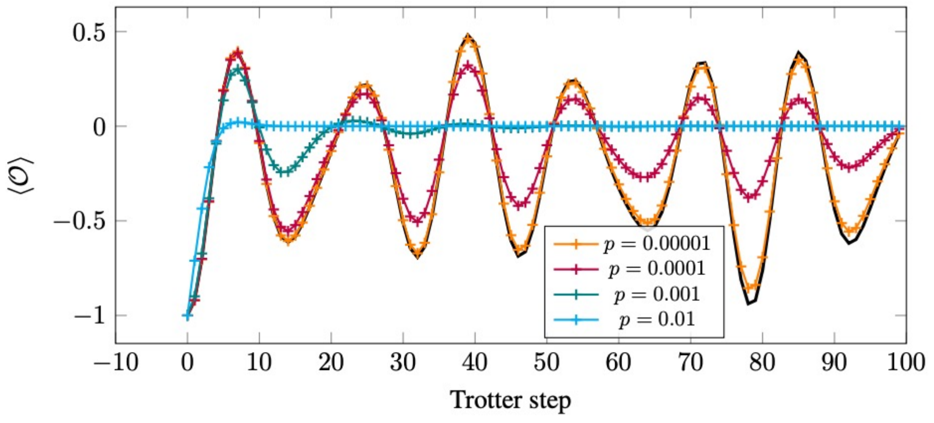


[Derby Klassen, Phys. Rev. B 104, 035118 (2021)]

Metric

How to assign a score to an output of the quantum computer?

Define a **distance** between the measured values and the exact value with a **physical** meaning.



On a quantum computer, expectation values must be **averaged over shots**. A finite number of shots comes with **statistical noise**. If statistical noise is higher than the **hardware noise** (due to imperfections), the hardware noise cannot be detected.

We can define a physical score by *the time that a perfect hardware would take to certify* (with say 3 standard deviations) *that the output of the tested hardware is biased*.

The “time” is measured in the total number of two-qubit gates implemented (number of two-qubit gates per circuit × number of shots).

Metric

Example

- Alice runs the benchmark protocol with 500 two-qubit gates on her quantum computer, and measures an expectation value 0.35 with negligible shot noise.
- We classically compute the exact value 0.4 with standard deviation 0.2 per shot.
- Let's imagine Bob doesn't know how to compute the exact value classically, but instead has access to a perfect quantum computer. Bob would need to run at least 144 shots on his perfect quantum computer to be certain (by 3 standard deviations) that Alice's quantum computer is imperfect.
- This means Bob would have to implement at least 72,000 two-qubit gates on his perfect quantum computer. This is the score of Alice's quantum computer. Before implementing this many gates, Alice's quantum computer is statistically compatible with a perfect quantum computer.

Benchmark protocol features

Summary

- ✓ **Scalable**: runtime is polynomial in system size
- ✓ **Application-oriented**: directly evaluates how well fermionic many-body systems can be simulated
- ✓ **Architecture-agnostic**: the 2D geometry is adapted both to all-to-all coupled quantum computers and grid-like quantum computer architectures
- ✓ **Interpretable**: outputs a single number with a physical, easy-to-interpret meaning

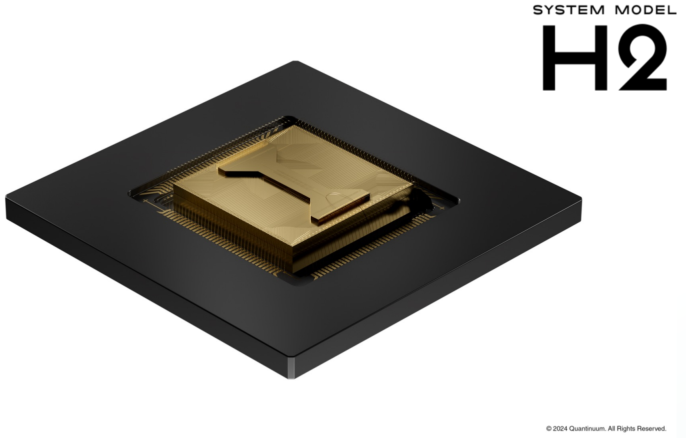
[Granet Dreyer, arXiv:2503.04298]

Hardware implementation

on Quantinuum's H2 ion-trap device

We implemented (part of) the benchmark protocol on our H2 trapped-ion system.

- Hosts 56 all-to-all coupled qubits.
- One-qubit gate fidelity 99.998%.
- Native two-qubit gate $e^{i\theta ZZ}$ with around 99.9% fidelity.



[Moses et al, Phys. Rev. X 13, 041052 (2023)]

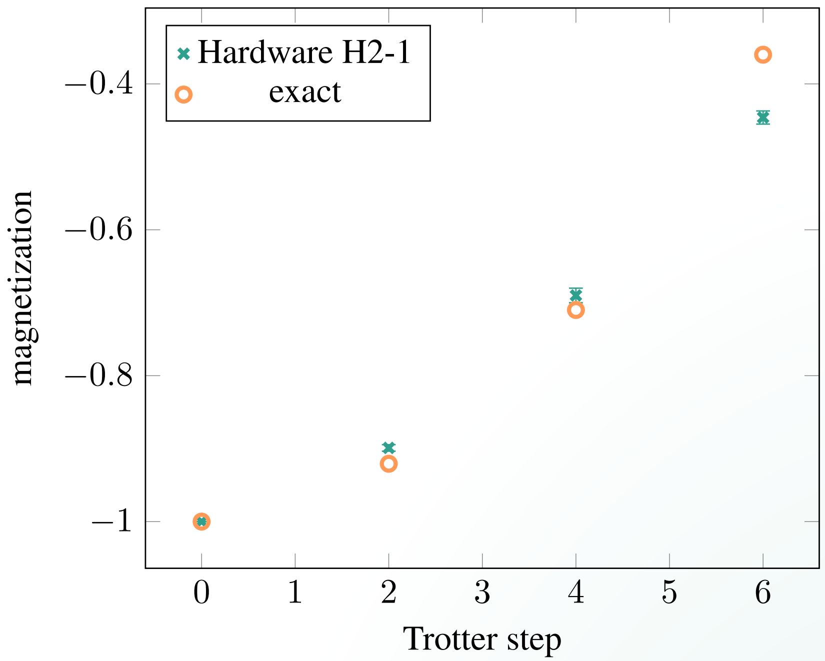
We simulated two spin types on a 4×4 lattice (one spin type=24 qubits).

We implemented 2, 4 and 6 Trotter steps.

Hardware implementation

Results

Trotter step	Number of TQ gates	Relative error	Number of shots to distinguish	Score
2	546	2.4% +/- 0.4%	197	107,562
4	1058	2.8% +/- 1.4%	1125	1,190,250
6	1586	23% +/- 2.5%	49	77,714

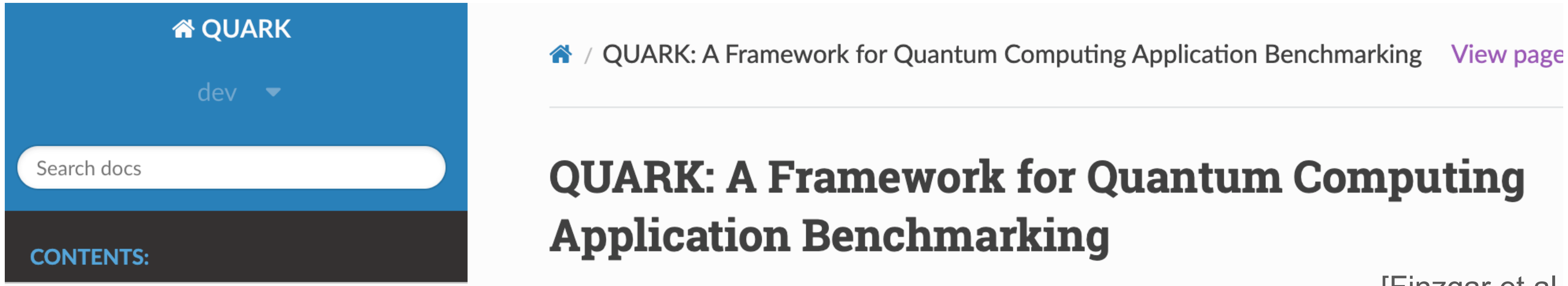


QUARK implementation

Circuits to download

The benchmark has been implemented in QUARK, a framework for quantum computing application benchmarking.

QUARK



[Finzgar et al, IEEE QCE2022]

You can implement it directly on your machine.

Thank you

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