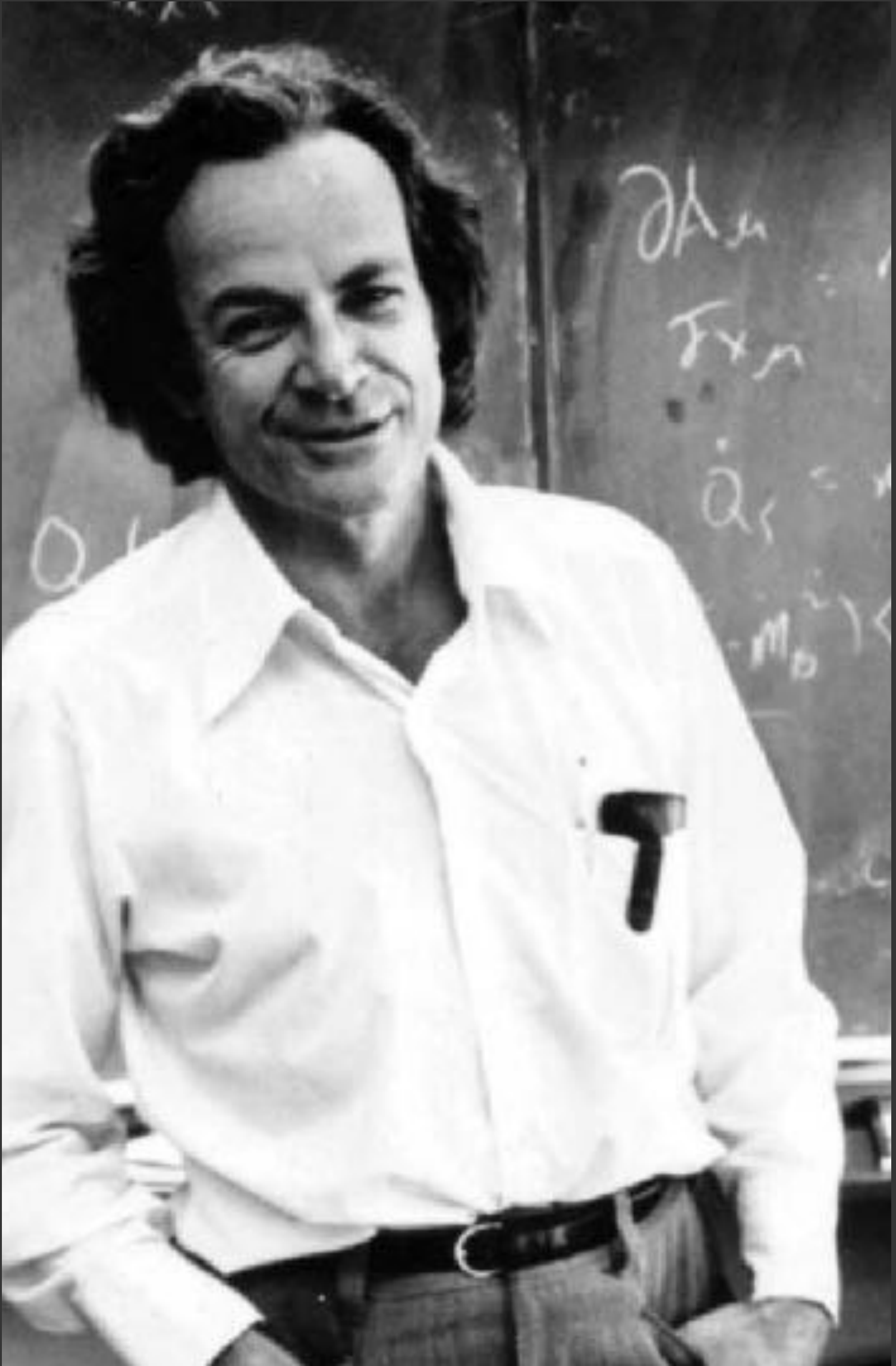
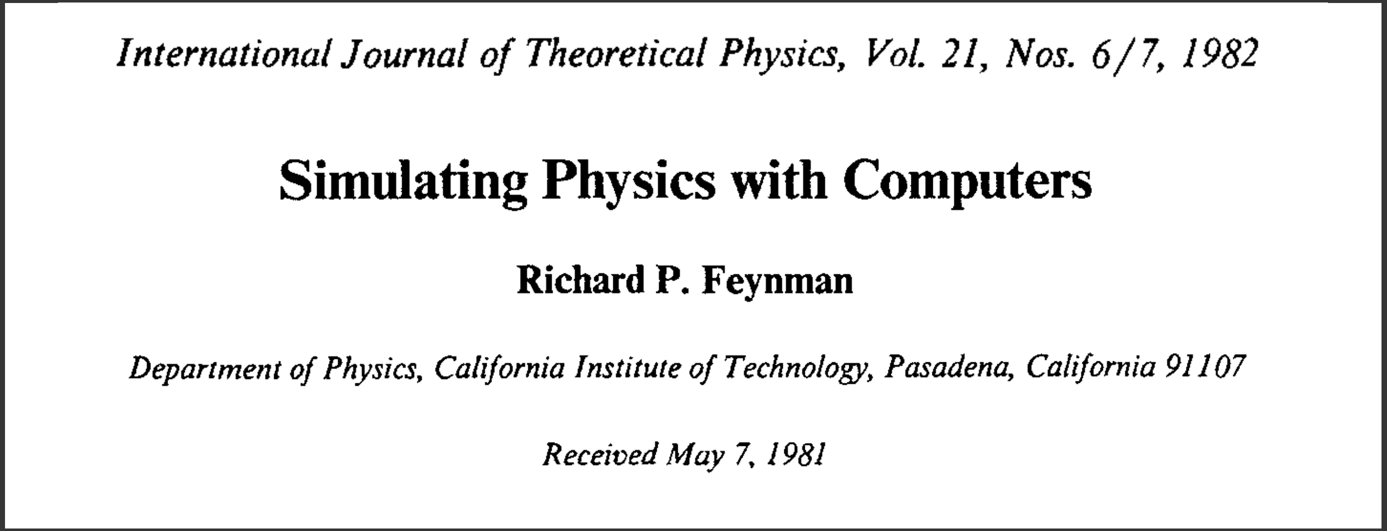
Microsoft

Accelerating QMC on quantum computers

Matthias Troyer





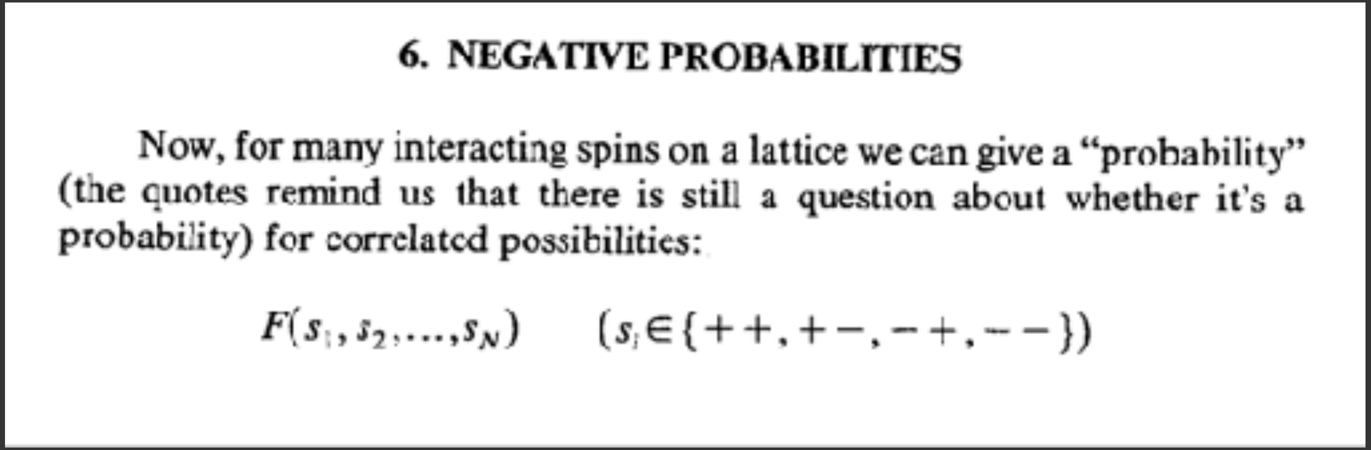
International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981



6. NEGATIVE PROBABILITIES

Now, for many interacting spins on a lattice we can give a "probability" (the quotes remind us that there is still a question about whether it's a probability) for correlated possibilities:

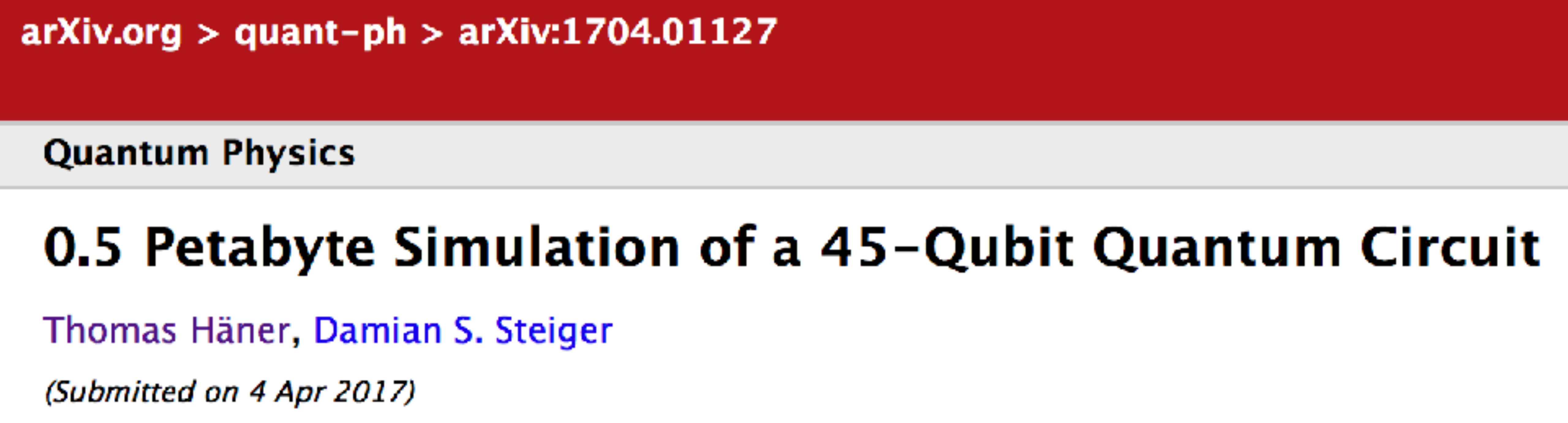
$$F(s_1, s_2, \ldots, s_N) \qquad (s_i \in \{++, +-, -+, --\})$$

Feynman proposed to use quantum computers to simulate quantum physics

Simulating quantum computers on classical computers

Simulating a quantum gate acting on N qubits needs $O(2^N)$ memory and operations

Qubits	Memory	Time for one operation
10	16 kByte	microseconds on a smartwatch
20	16 MByte	milliseconds on smartphone
30	16 GByte	seconds on laptop
40	16 TByte	seconds on cluster
50	16 PByte	minutes on top supercomputers?
60	16 EByte	hours on exascale supercomputer?
70	16 ZByte	days on hypothetical future supercomputer?
…	…	…
250	size of visible universe	age of the universe



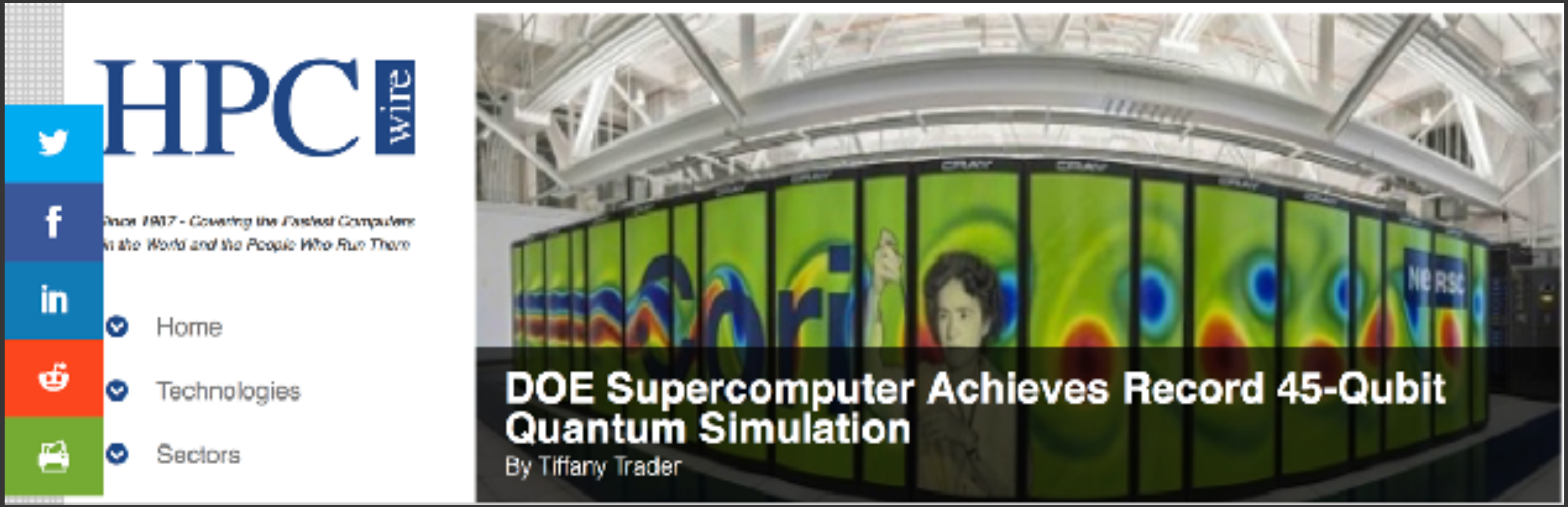
arXiv.org > quant-ph > arXiv:1704.01127

Quantum Physics

0.5 Petabyte Simulation of a 45-Qubit Quantum Circuit

Thomas Häner, Damian S. Steiger

(Submitted on 4 Apr 2017)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DOE Supercomputer Achieves Record 45-Qubit Quantum Simulation

By Tiffany Trader

Preparing the ground state

On a classical computer

Imaginary time projection

$$\left|\Psi_{GS}\right\rangle = \lim_{\tau\to\infty} e^{-\tau H}\left|\Psi_T\right\rangle$$

Power method or other iterative eigensolver

$$\left|\Psi_{GS}\right\rangle = \lim_{n\to\infty}(H-\Lambda)^n\left|\Psi_T\right\rangle$$

On a quantum computer

~~Imaginary time evolution~~

~~Power method~~

Unitary operations + measurements:

prepare trial state

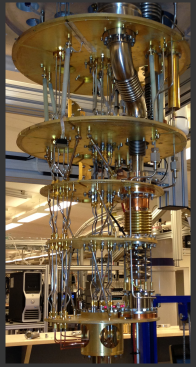
$$\left|\Psi_T\right\rangle$$

projectively measure energy

$$\left|\Psi_T\right\rangle \to \left|\phi_n\right\rangle \text{ with } H\left|\phi_n\right\rangle = E_n\left|\phi_n\right\rangle$$

$$\left|\phi_n\right\rangle \text{ picked with propability } \left|\left\langle\phi_n\middle|\Psi_T\right\rangle\right|^2$$

obtain the ground state if
the ground state energy was measured



Quantum phase estimation

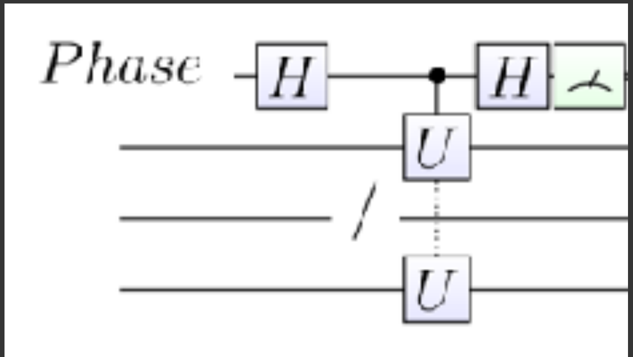
Energy can be measured through the phase of a wave function after unitary time evolution

$$U\left|\phi_n\right\rangle \equiv e^{-iHt}\left|\phi_n\right\rangle = e^{-iE_nt}\left|\phi_n\right\rangle = e^{-i\phi}\left|\phi_n\right\rangle$$

We can only measure relative phases, thus do a controlled evolution

$$\left|0\right\rangle\left|\phi_n\right\rangle \to \frac{1}{\sqrt{2}}\left(\left|0\right\rangle+\left|1\right\rangle\right)\left|\phi_n\right\rangle \to \frac{1}{\sqrt{2}}\left(\left|0\right\rangle\left|\phi_n\right\rangle+U\left|1\right\rangle\left|\phi_n\right\rangle\right) = \frac{1}{\sqrt{2}}\left(\left|0\right\rangle+e^{-i\phi}\left|1\right\rangle\right)\left|\phi_n\right\rangle \to \frac{1}{2}\left((1+e^{-i\phi})\left|0\right\rangle+(1-e^{-i\phi})\left|1\right\rangle\right)\left|\phi_n\right\rangle$$

Measure the ancilla qubit to obtain the phase



Solving quantum chemistry on a quantum computer

1. Select a finite (generally non-orthogonal) basis set

2. Perform a Hartree-Fock calculation to

   get an approximate solution

   get an orthogonal basis set

3. Find the true ground state of the Hamiltonian in this new basis set

$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r$$

exact classical approach: full-configuration interaction
exponential complexity!

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4. Prepare a good guess for the ground state

5. Perform quantum phase estimation to

   get the ground state wave function and energy

Representing fermion terms by quantum circuits

Map the occupation of each spin-orbital to the states of one qubit

$$|0\rangle = |\uparrow\rangle \qquad |1\rangle = |\downarrow\rangle$$

Density operators get mapped to Pauli matrices

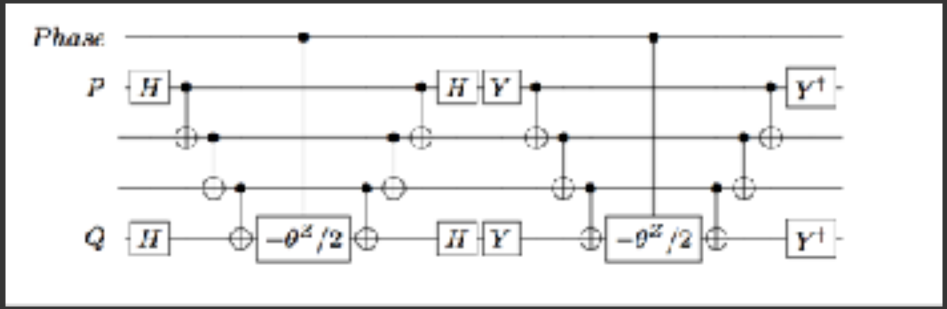
$$n_i = \frac{1}{2}\left(1 - \sigma_i^z\right)$$

Hopping terms get mapped to spin flips with Jordan-Wigner strings

$$c_p^\dagger c_q = \sigma_p^- \prod_{i=p+1}^{q-1} \sigma_i^z \sigma_p^+$$

Time evolution gets mapped to circuits built from unitary gates

$$e^{-i\theta\left(c_p^\dagger c_q + c_q^\dagger c_p\right)} =$$



Simulating time evolution on quantum computers

There are O(*N*⁴) interaction terms in an *N*-electron system

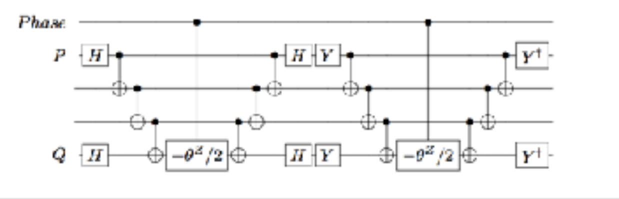
$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r \equiv \sum_{m=1}^{M} H_m$$

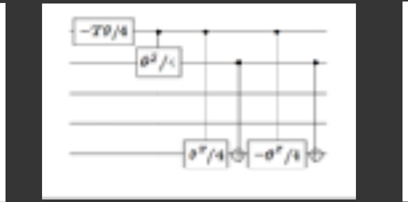
$M = O(N^4)$ terms

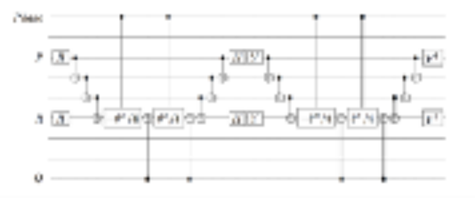
We need to evolve separately under each of them

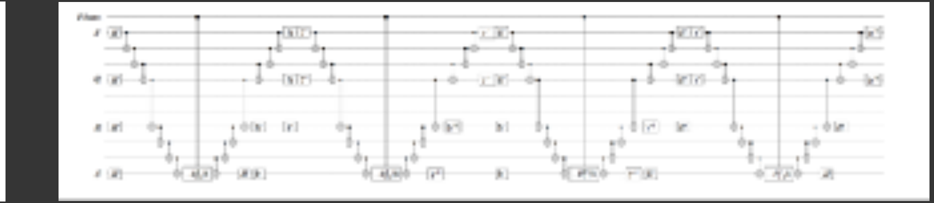
$$e^{-i\Delta t H} \approx \prod_{m=1}^{M} e^{-i\Delta\tau H_m}$$

Efficient circuits available for each of the *N*⁴ terms









Runtime estimates turn out to be O(*NM*²) = *O*(*N*⁹)

It's efficient since it's polynomial!

The polynomial time quantum shock

Estimates for a benchmark molecule: Fe_2S_2 with 118 spin-orbitals

Gate count	10^{18}
Parallel circuit depth	10^{17}
Run time @ 100ns gate time	300 years

We cannot declare victory proving the existence of polynomial time algorithms

We need quantum software engineers to develop better algorithms and implementations

The result of quantum software optimization

Estimates for a benchmark molecule: Fe_2S_2 with 118 spin-orbitals

Gate count	10^{18}
Parallel circuit depth	10^{17}
Run time @ 100ns gate time	300 years

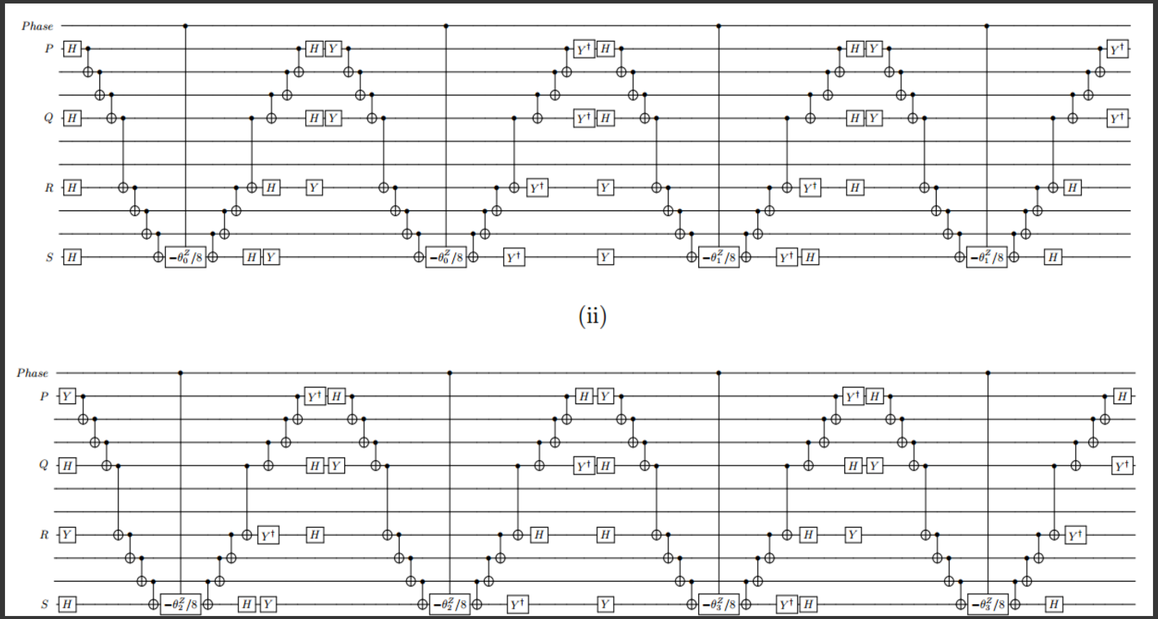
Reduced gate count	10^{11}
Parallel circuit depth	10^{10}
Run time @ 100ns gate time	20 minutes

Attempting to reduce the horrendous runtime estimates we achieved
Wecker *et al.*, PRA (2014), Hastings *et al.*, QIC (2015), Poulin *et al.*, QIC (2015)

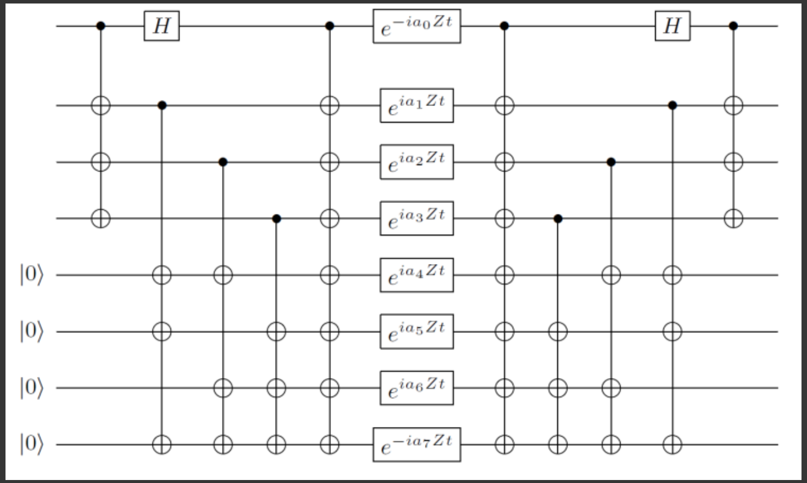
Reuse of computations:	O(*N*) reduction in gates
Parallelization of terms:	O(*N*) reduction in circuit depth
Optimizing circuits:	4x reduction in gates
Smart interleaving of terms:	10x reduction in time steps
Multi-resolution time evolution:	10x reduction in gates
Better phase estimation algorithms:	4x reduction in rotation gates

Improvements in algorithms

Original circuit



Improved circuit



Guessing a good trial state

Mean field approximation

Hartree-Fock

Density functional theory

Variational approaches: fit parameters in variational ansatz

Configuration-Interaction

Variational Monte Carlo McMillan, Phys. Rev (1965)

Tensor network methods (e.g. DMRG) White, Phys. Rev. Lett. (1992)

Neural network states Carleo & Troyer, Science (2017)

Preparing a good trial state

Adiabatic evolution from a simple initial Hamiltonian H_0 with known ground state to the desired Hamiltonian H_1

$$H(s) = (1 - s)H_0 + sH_1$$

Good starting Hamiltonians

- Mean-field approximation (with right broken symmetry)
- Non-interacting particles (in the right symmetry sector)

Variational quantum eigensolvers

Perform variational quantum Monte Carlo on wave functions prepared by a quantum circuit

$$\left|\Psi\right\rangle = U(\lambda_1,\ldots,\lambda_N)\left|0\right\rangle$$

Allows classes of wave functions to be efficiently evaluated that are hard to evaluate classically, such as unitary coupled cluster

Peruzzo et al, Nature Comm. (2014)

Reducing sampling errors

Error in Monte Carlo sampling $\varepsilon \sim \frac{1}{\sqrt{t}}$

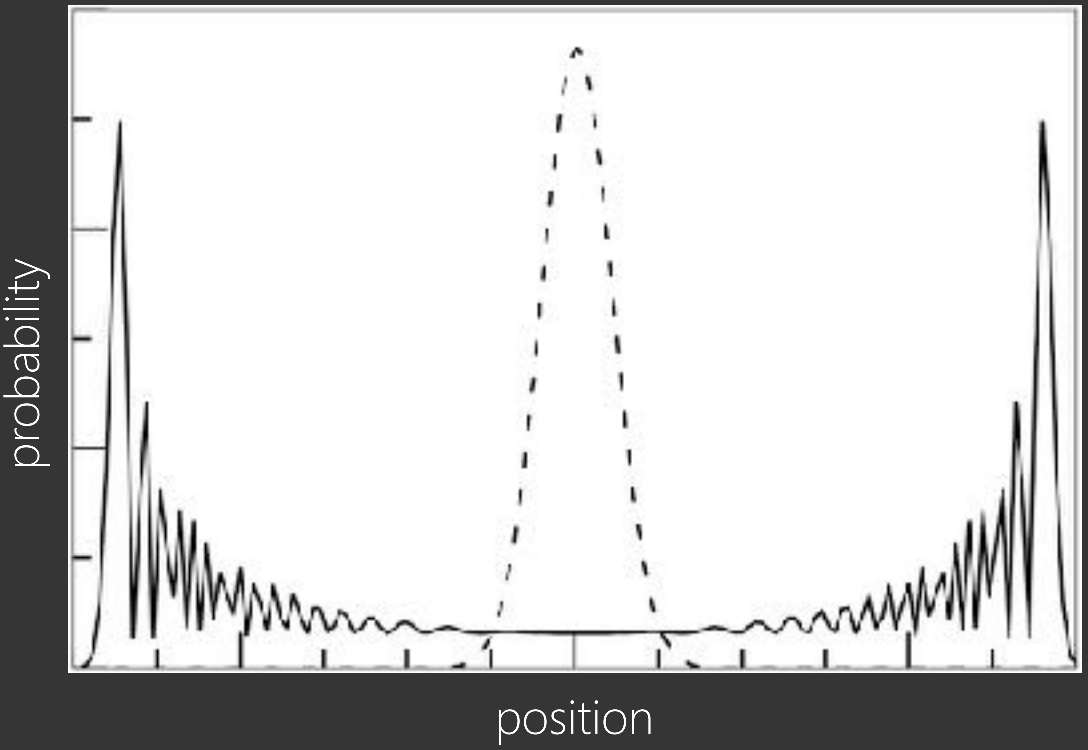
Error in quantum phase estimation (QPE) $\varepsilon \sim \frac{1}{t}$

Quantum amplitude estimation uses QPE to measure expectation values. (Brassard *et al*, 2002) $\langle A \rangle = \langle \Psi | A | \Psi \rangle$ $\varepsilon \sim \frac{1}{t}$

Encode distribution to be samples in the wave function

Accelerating Monte Carlo through Quantum Walks

Markov processes can be implemented as quantum walks with quadratic and sometimes exponential acceleration in the mixing times.



Szegedy's quantum walk for MCMC

Map a Markov process with transition matrix T_{xy} into a quantum circuit

$$X|x\rangle|0\rangle = \sum_y \sqrt{T_{xy}}\,|x\rangle|y\rangle$$

The quantum walk operator W has the equilibrium distribution as eigenvector with eigenvalue 1

$$W = X^\dagger P X P R P X^\dagger P X R$$

$$P|x\rangle|y\rangle = |y\rangle|x\rangle$$

$$R = \left[Id - |0\rangle\langle 0| \right] \otimes Id$$

Solving the sign problem in QMC

Monte Carlo sampling with the quantum Metropolis algorithm

- Use a unitary update + phase estimation to propose a new energy eigenstate
- Accept or reject according to the Metropolis algorithm
- Solves the sign problem of QMC by working with energy eigenstates

Temme et al, Nature (2011)

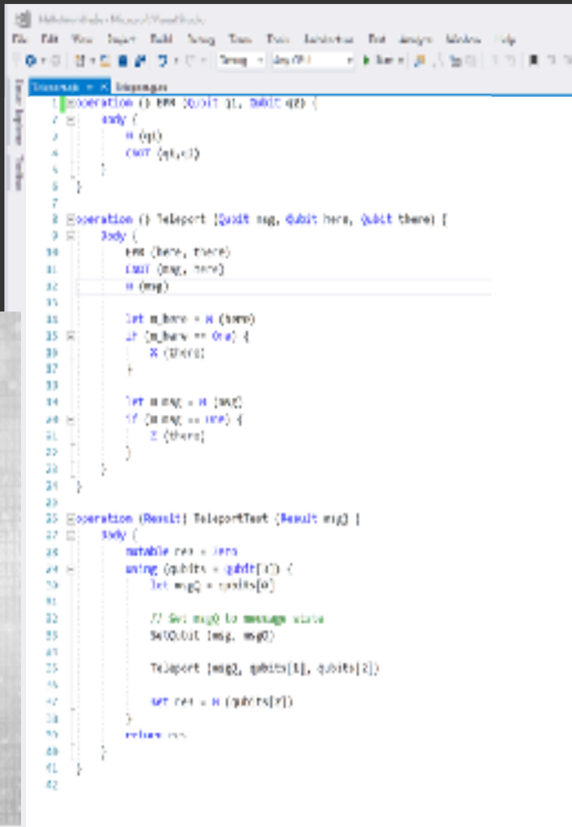
It is time to start writing quantum software

Invent new quantum algorithms

Explore quantum applications

Determine resources and optimize quantum code

Co-design quantum hardware and software



```
operation () EPR (Qubit q1, Qubit q2) {
    body {
        H (q1)
        CNOT (q1,q2)
    }
}

operation () Teleport (Qubit msg, Qubit here, Qubit there) {
    body {
        EPR (here, there)
        CNOT (msg, here)
        H (msg)

        let m_here = M (here)
        if (m_here == One) {
            X (there)
        }

        let m_msg = M (msg)
        if (m_msg == One) {
            Z (there)
        }
    }
}

operation (Result) TeleportTest (Result msg) {
    body {
        mutable res = Zero
        using (qubits = qubit[3]) {
            let msgQ = qubits[0]

            // Set msgQ to message state
            SetQubit (msg, msgQ)

            Teleport (msgQ, qubits[1], qubits[2])

            set res = M (qubits[2])
        }
        return res
    }
}
```