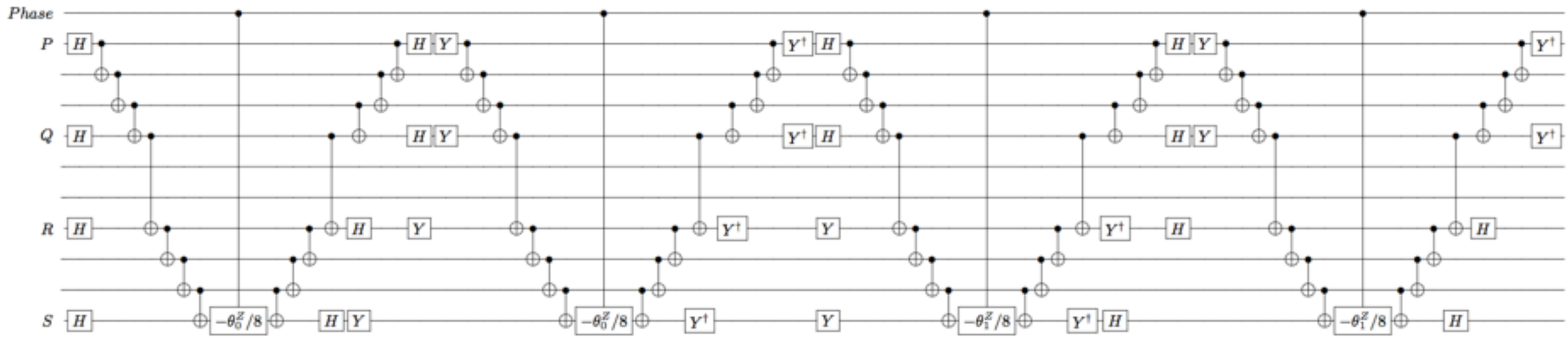


Solving strongly correlated systems on a quantum computer

Matthias Troyer - Station Q Zurich, ETH Zurich

Classical computers have come a long way

Antikythera mechanism

astronomical positions

(100 BC)

Kelvin's harmonic analyzer

prediction of tides

(1878)

digital devices

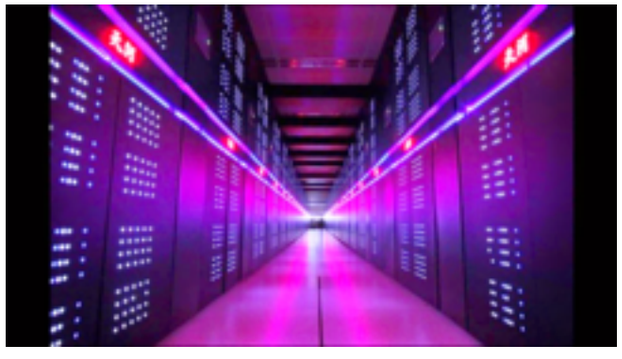
more complex

but general purpose

and error correcting

ENIAC

(1946)



天河-2

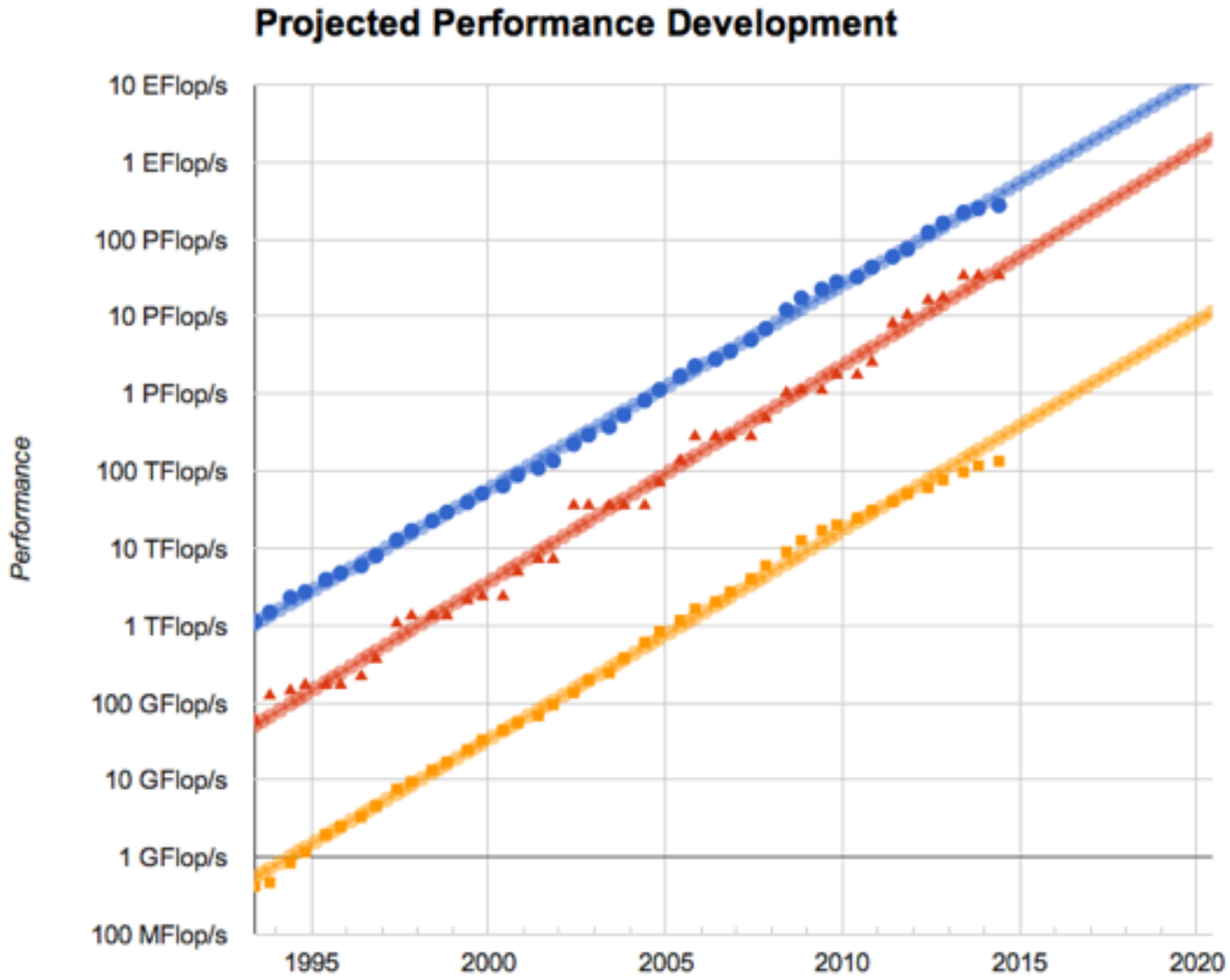
(2013)

analog devices

conceptually simple

calibration and scaling problems

How long will Moore's law continue?



CPU cores:	1024	8'192	3'120'000	Amdahl's law: 99.99993% parallel
Power:	1 MW	3 MW	20 MW	1 MW ≈ 1 M€ / year

HPC 2014

HIGH PERFORMANCE COMPUTING

FROM CLOUDS AND BIG DATA TO EXASCALE AND BEYOND

Argonne NATIONAL LABORATORY

Enabling technologies for beyond exascale computing

Paul Messina

Director of Science

Argonne Leadership Computing Facility

Argonne National Laboratory

July 9, 2014

Cetraro

What is “Beyond Exascale Computing?”

- **We are not referring to 10**21 flops**
- **“Beyond exascale” systems as we are defining them will be based on new technologies that will finally result in the much anticipated (but unknown) phase change to truly new paradigms/methodologies.**

Quantum computing

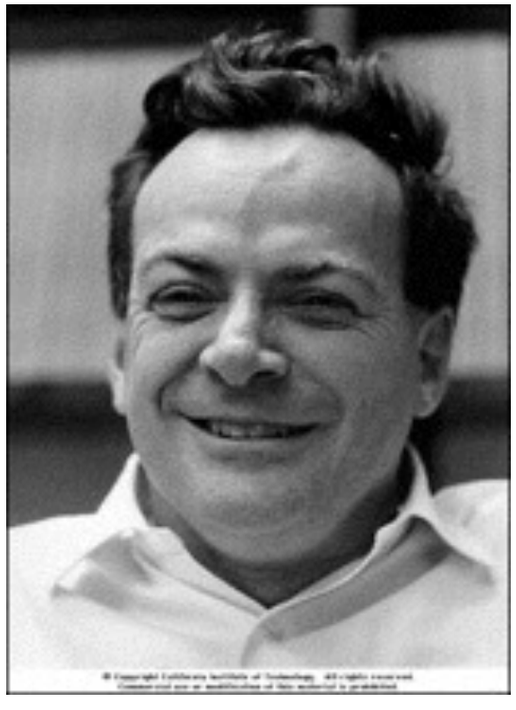
International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

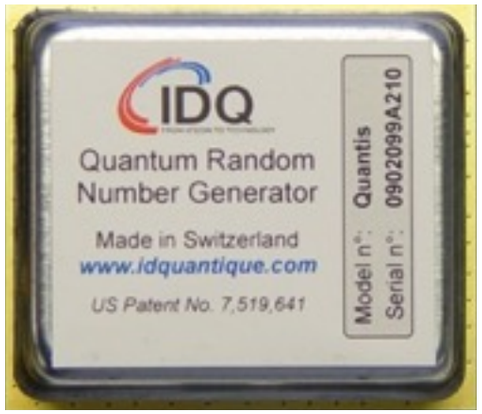
Richard P. Feynman

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

Received May 7, 1981



Beyond exascale computing: quantum devices



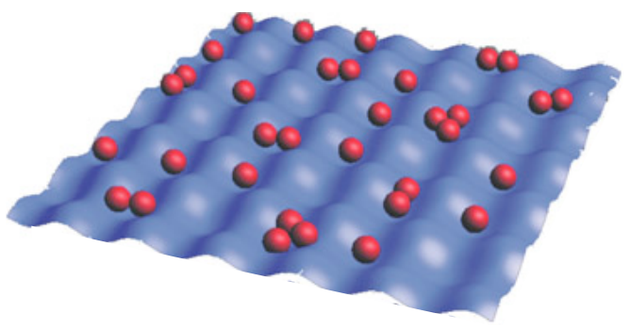
Quantum random numbers

perfect randomness

Quantum encryption

secure communication

Quantum computers?



Analog quantum simulators

solve quantum models

Quantum annealer

solve hard optimization problems?

Simulating quantum computers

- Need 2^N complex numbers to store the wave function of N qubits
- $O(2^N)$ classical operations to perform a quantum gate on N qubits

Qubits	Memory	Time for one gate
10	16 kByte	microseconds on a smart watch
20	16 MByte	milliseconds on smartphone
30	16 GByte	seconds on laptop
40	16 TByte	minutes on supercomputer
50	16 PByte	days on top supercomputer
60	16 EByte	long long time
80	size of visible universe	age of the universe

The best qubits: ion traps

- Use the motional states of well isolated ions to encode a qubit
  - up to 20 qubits (Innsbruck)
  - life time of hours when isolated
  - 10 µs gate times
  - survive about 100 gate operations

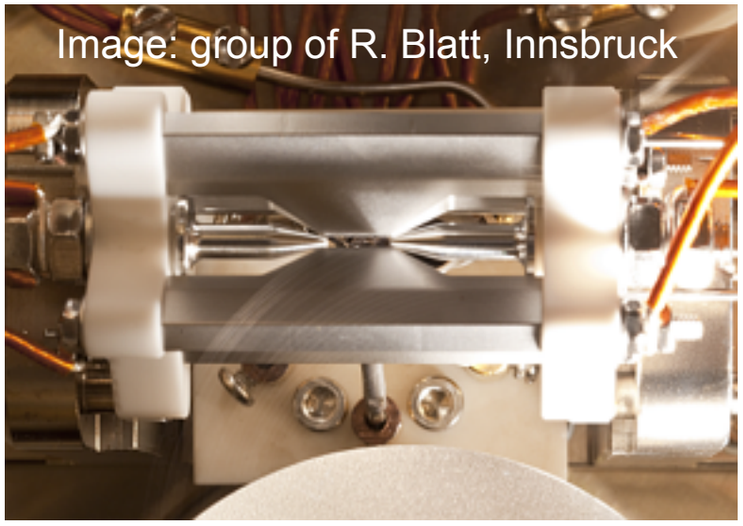
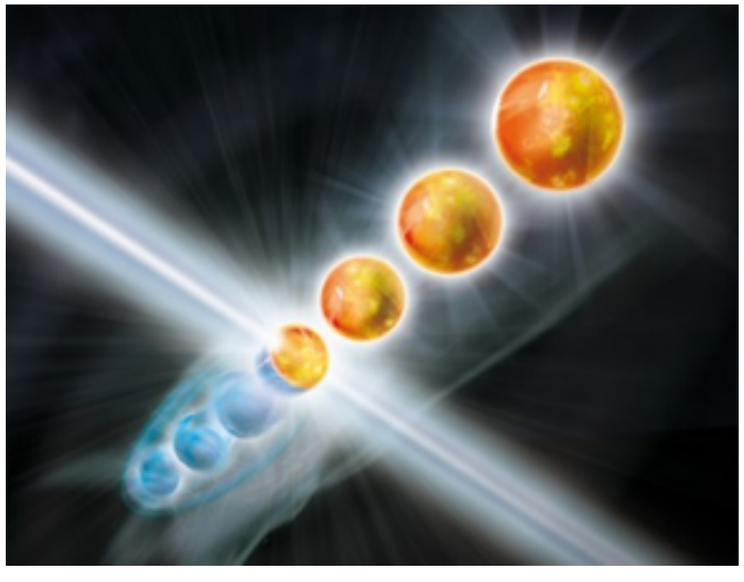


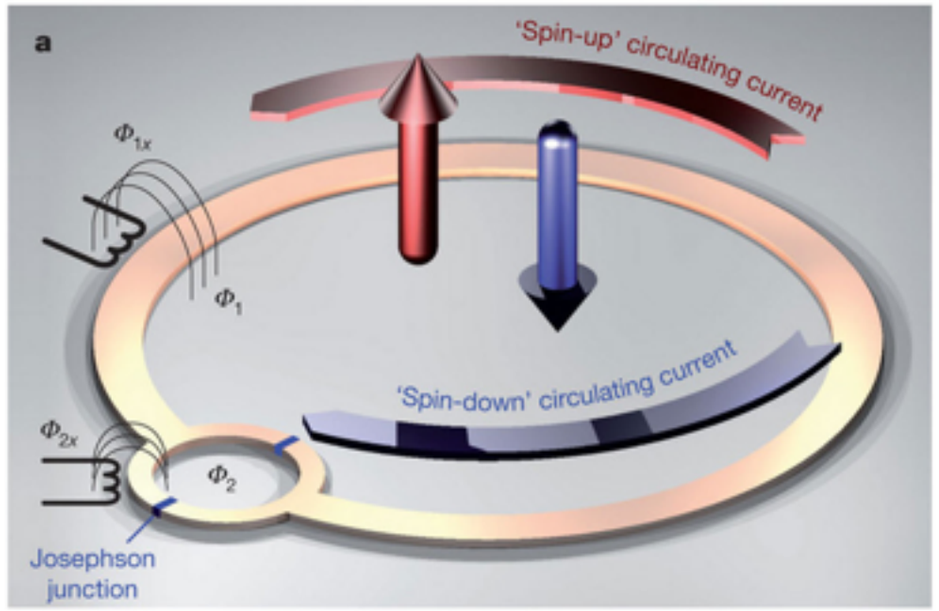
Image: group of R. Blatt, Innsbruck

- Advantages and disadvantages
  - Well isolated from environment and thus very long lived
  - Relatively slow
  - Hard to scale beyond O(20) qubits

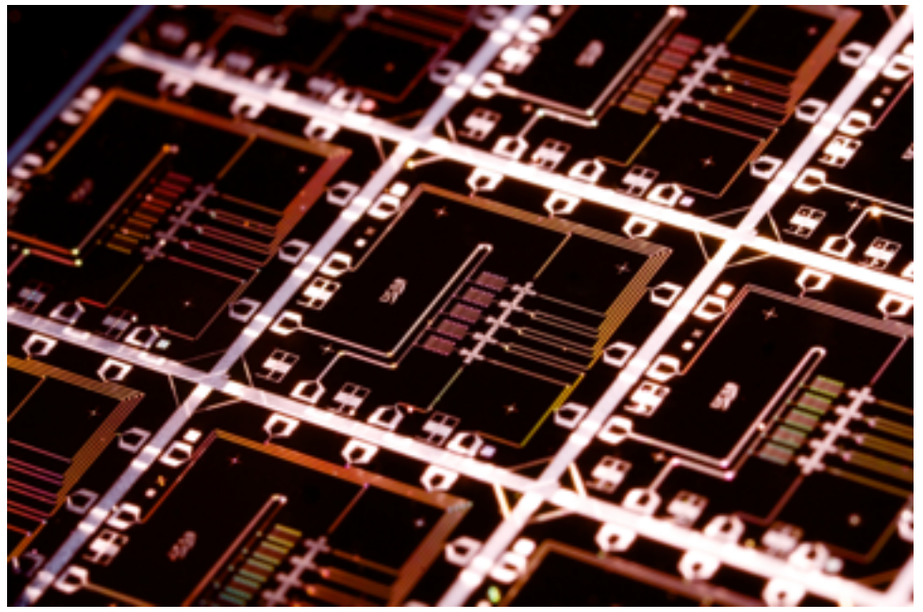


Superconducting qubits

- Use superconducting current loops to encode a qubit
- State of the art
  - O(10) qubits (UCSB, IBM)
  - life time of 100 µs
  - 10 ns gate times
  - survive about 100 gate operations

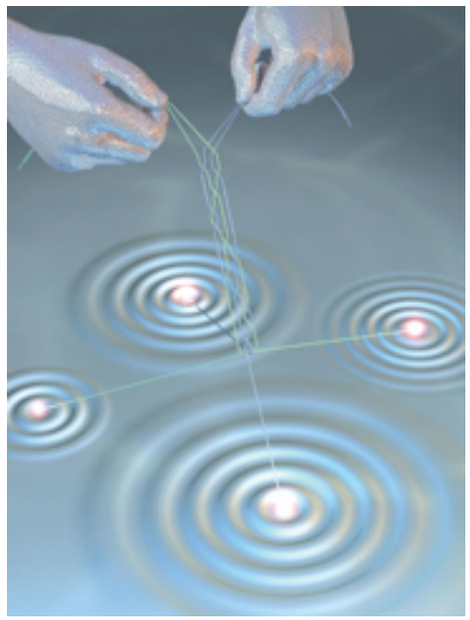


- Advantages and disadvantages
  - scalable
  - fast
  - can be built in semiconductor foundries
  - but lots of coupling to the chip and thus short lifetimes

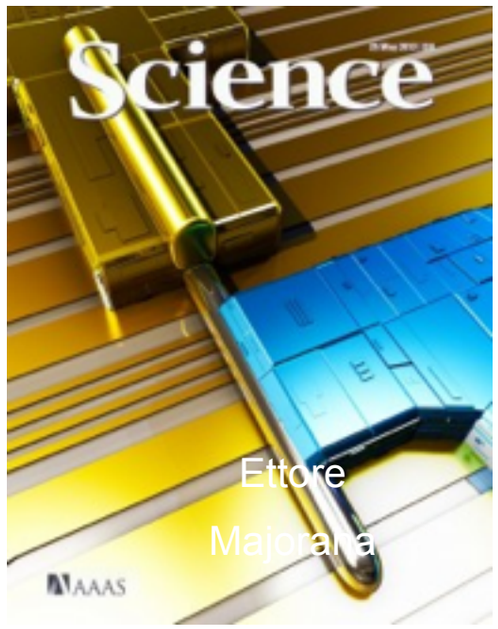


Topological qubits (Microsoft and TU Delft)

- Encode the qubit in a topological property of a quantum state
  - Intrinsic protection due to topology
  - No local noise can detect or destroy the state
  - No expensive error correction needed



- Most promising: Majorana particles (Microsoft and TU Delft)
  - may exist at ends of superconducting nanowires
  - string evidence but not yet confirmed
  - Operations done by “braiding” isolated particles



Ettore Majorana

Quantum computing beyond exa-scale

What are the important applications …

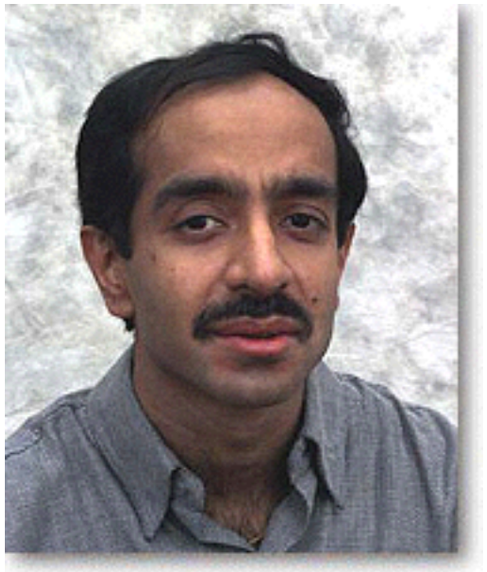
… that we can solve on a quantum computer …

… but not special purpose post-exa-scale classical hardware that we may build in ten years?

Grover search

- Search an unsorted database of N entries in $\sqrt{N}$ time
- Rare case of provable quantum speedup given an oracle

- However, the oracle needs to be implemented!
  - N-entry database needs at least O(N) hardware resources to store the data
  - Can perform the same search classically in log(N) time with special purpose hardware



- Grover search is only useful if the database can be calculated on the fly
- Are there important real-world applications?

Shor's algorithm for factoring

- Factoring is hard classically: O(exp($N^{1/3}$)) time for N bit - numbers

5369396836426911946079505415332600518604181838930231166202317318847061358416977798124777555435596464904452615804209177029240538156141035272554197625377862483029051809615050127043414927261020411423649694630967091077171430279795022115120241679622849447805650987368350247829683054309216276674509735105639240298977591783205062161915884859331945476609848287512883478098897975108372321438198667838135056716743636376259314981677010612529720589301303706515881099466219525234349036065726516132873421237667900245913537253744354928238018040554845306796065865605354860834270732796989421041371044010901319172800167360587954169579897308037630097009691131029791433294622359167226074868486707285279145057386192915950796

- But is polynomial time on a quantum computer
  - O(N^3) using minimal number of $2N$+3 qubits
  - O(N^2) using O(N) qubits
  - O(N) using O(N^2) qubits

- Shor's algorithm suddenly made quantum computing interesting

Shor's algorithm and encryption

- Shor's algorithm can be used to crack RSA encryption
  - assuming 10 ns gate time and minimal number of 2N+3 qubits
  - much faster (seconds) when using more qubits

RSA	cracked in	CPU years	Shor
453 bits	1999	10	1 hour
768 bits	2009	2000	5 hours
1024 bits		1000000	10 hours

- But use of quantum computers to crack RSA is limited since we can anytime switch to post-quantum encryption
  - quantum cryptography
  - lattice based cryptography

Quantum page rank

PRL 108, 230506 (2012) PHYSICAL REVIEW LETTERS week ending 8 JUNE 2012

Adiabatic Quantum Algorithm for Search Engine Ranking

Silvano Garnerone,[1,2,5] Paolo Zanardi,[2,5] and Daniel A. Lidar[2,3,4,5]

[1]*Institute for Quantum Computing, University of Waterloo, Waterloo, ON N2L 3G1, Canada*
[2]*Department of Physics & Astronomy, University of Southern California, Los Angeles, California 90089, USA*
[3]*Department of Electrical Engineering, University of Southern California, Los Angeles, California 90089, USA*
[4]*Department of Chemistry, University of Southern California, Los Angeles, California 90089, USA*
[5]*Center for Quantum Information Science & Technology, University of Southern California, Los Angeles, California 90089, USA*

(Received 25 October 2011; published 4 June 2012)

We propose an adiabatic quantum algorithm for generating a quantum pure state encoding of the PageRank vector, the most widely used tool in ranking the relative importance of internet pages. We present extensive numerical simulations which provide evidence that this algorithm can prepare the quantum PageRank state in a time which, on average, scales polylogarithmically in the number of web pages. We argue that the main topological feature of the underlying web graph allowing for such a scaling is the out-degree distribution. The top-ranked $\log(n)$ entries of the quantum PageRank state can then be estimated with a polynomial quantum speed-up. Moreover, the quantum PageRank state can be used in ''q-sampling'' protocols for testing properties of distributions, which require exponentially fewer measurements than all classical schemes designed for the same task. This can be used to decide whether to run a classical update of the PageRank.

Complexity of quantum page rank

- log(*N*) qubits are sufficient, but are not practical
- *N* qubits allow for a straightforward unary encoding

- Page rank then solved by adiabatic evolution of a spin model

$$H(s) = \sum_{i=1}^{n} h(s)_{ii} \sigma_i^+ \sigma_i^- + \sum_{i<j}^{n} h(s)_{ij} \left(\sigma_i^+ \sigma_j^- + \sigma_j^+ \sigma_i^- \right),$$

- Needs O(N^a) time with a ≈ 0.2…1
  when implementing N^2 couplings in parallel
  using O(N^2) hardware resources

- Classical page rank needs O(1) matrix-vector multiplications,
  each of complexity O(*dN*) where *d* is the mean number of links

Compare to classical hardware

	Quantum custom hardware	Classical general purpose	Classical custom hardware
Serial time complexity	O(N^2 polylog(N))	O(dN log(N))	O(dN)
Memory required	O(N) qubits	O(N) bits	O(N) bits
Parallel time complexity	O($N^{0.2}$) – O(N)	O($N^{1/3}$) on 3D crossbar network	O(log(N))
Hardware required	O(N^2)	O(dN)	O(dN)

- Quantum speedup vanishes when comparing parallel quantum hardware to parallel special purpose classical hardware
- Classical hardware requirements increase slower classically than quantum

Solving linear systems of equations

Harrow, Hassidim, Lloyd, PRL (2009)

- Solve linear system $Ax=b$ in $\log(N)$ time
- Requirements
  - Only $\log(N)$ bits of the answer are needed
  - Problem is well conditioned
  - Time evolution using the matrix A can be implemented efficiently

$$e^{-iAt}\left|b\right\rangle$$

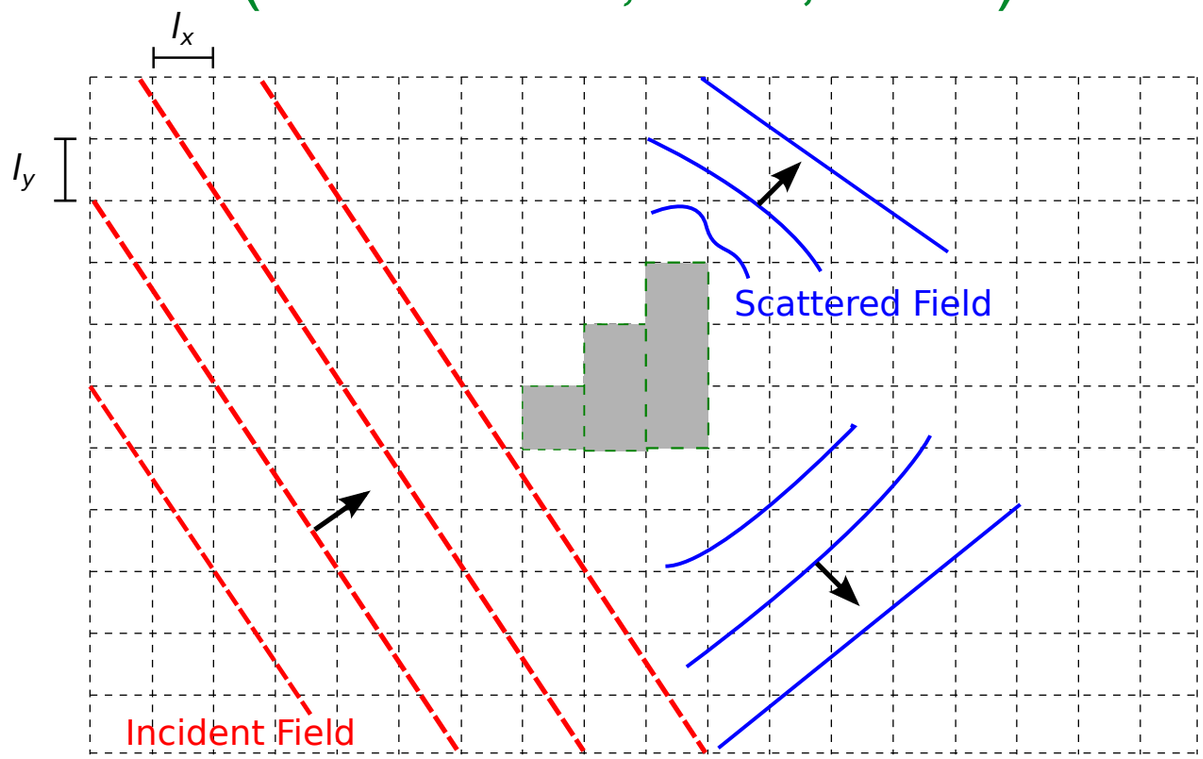
Implementing a general time evolution

- In general we always need O(N^2) gates if matrix A has N^2 different entries
- Lloyd, Mohseni and Rebentrost (Nature Physics 2014) propose an O(log(N)) implementation using QRAM to store square root of the matrix
  - needs O(N^2) gates and qubits to implement the QRAM
  - needs O(N^3) effort in classical preparation to calculate the square root
- How does it compare to classical approaches?
  - Gaussian elimination solves a linear system in O(N^3) time using O(N^2) memory
  - Using O(N^2) classical hardware we can do a matrix-vector multiplication in O(log(N)) time and solve the problem iteratively
- Furthermore, using O(N^2) classical hardware we can classically emulate any quantum algorithms acting on 2 log N qubits.

Solving linear systems of equations efficiently

- Quantum speedup can only be realized if the evolution exp(-*iAt*) can be implemented using a short circuit, i.e. it does not depend on lots of data

- Electromagnetic wave scattering problem (Clader *et al,* PRL, 2013)
  - finite difference discretization
  - represent shapes by splines



- Competitive with classical hardware for runtimes beyond a millennium
  We need to speed this up and find better problems!

Quantum simulations on quantum computers

- R.P. Feynman,*Simulating Physics with Computers,* Int. J. of Theor. Phys., **21**, 467 (1982)
- S. Lloyd, *Universal Quantum Simulators,* Science **273**, 1073 (1996).
- D.S. Abrams and S. Lloyd*, Simulation of Many-Body Fermi Systems on a Universal Quantum Computer*, Phys. Rev. Lett. **79**, 2586 (1997)
- M.A. Nielsen and I.C. Chuang*, Quantum Computation and Quantum Information*, Cambridge University Press (2001)
- G. Ortiz *et al*., *Quantum algorithms for fermionic simulations*, Phys. Rev. A 64, 022319 (2001).
- R. Somma *et al*., *Simulating physical phenomena by quantum networks*, Phys. Rev. A **65**, 042323 (2002).
- Simulation of electronic structure Hamiltonians using quantum computers.
- J.D Whitfield, J. Biamonte and A. Aspuru-Guzik, *Simulation of electronic structure Hamiltonians using quantum computers,* Molecular Physics **109**, 735 (2011).
- Our papers: http://arxiv.org/find.quant-ph/1/AND+au:+Troyer+au:+Hastings+au:+Wecker/0/1/0/all/0/1/

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

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

4. Prepare a good guess for the ground state

5. Perform quantum phase estimation to
   - get the ground state wave function
   - get the ground state energy

Whitfield, Biamonte, Aspuru-Guzik
Molecular Physics (2011)

Solving quantum chemistry on a quantum computer

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

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   - get an approximate solution
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$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r$$

4a. Prepare the Hartree Fock wave function
4b. Adiabatically evolve from the Hartree-Fock Hamiltonian to the full one

5. Perform quantum phase estimation to
   - get the ground state wave function
   - get the ground state energy

Whitfield, Biamonte, Aspuru-Guzik
Molecular Physics (2011)

Time evolution under the Coulomb Hamiltonian

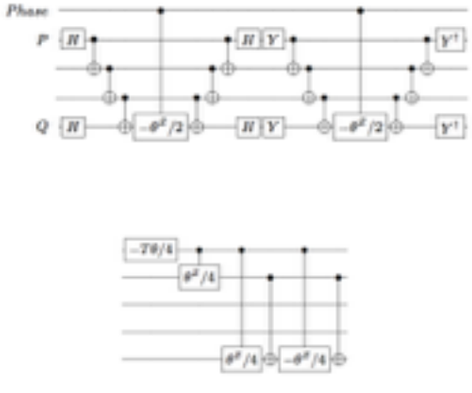
- Key ingredient: evolve the wave function under the Coulomb Hamiltonian

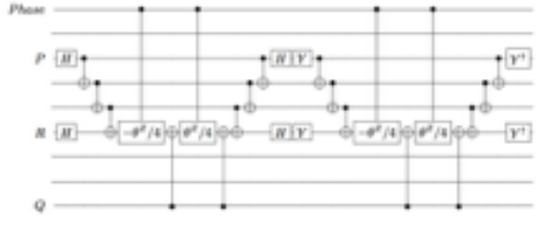
$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_r \equiv \sum_{m=1}^{M} H_m \qquad M = O(N^4) \text{ terms}$$

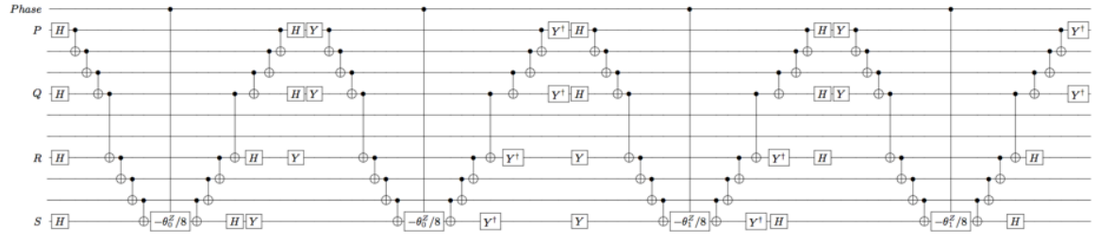
- Use Trotter breakup to implement time evolution
  Whitfield, Biamonte, Aspuru-Guzik, Molecular Physics (2011)

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

- Efficient circuits available for each of the $M=N^4$ terms







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

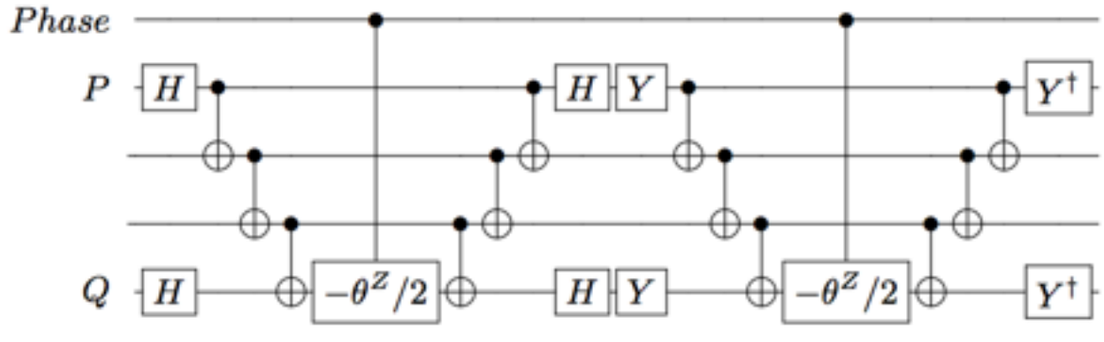
$$n_i = \frac{1}{2}\left(1 - \sigma_i^z\right)$$

- 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

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



Can quantum chemistry be performed on a small quantum computer?

Dave Wecker,[1] Bela Bauer,[2] Bryan K. Clark,[2,3] Matthew B. Hastings,[2,1] and Matthias Troyer[4]

[1] *Quantum Architectures and Computation Group, Microsoft Research, Redmond, WA 98052, USA*
[2] *Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA*
[3] *Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA*
[4] *Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

Phys. Rev. A **90**, 022305 (2014)

Can a classically-intractable problem be solved on a small quantum computer?

Can a classically-intractable problem be solved on a huge quantum computer?

Can a classically-intractable problem be solved on the largest imaginable quantum computer?

Solving a small non-trivial problem

- How many spin-orbitals do we need for an interesting problem?

Cuprate high-T_c superconductor	O(10000)
Active space of interesting reactions	200-400
Classically tractable by DMRG	≈ 70
Classically tractable by full-CI	≈ 50

- What accuracy do we need?

Wish of my chemistry colleague	0.1mHa - 1μHa
Modest goal	**1mHa**

Note that the total energies are of the order of 1kHa

We thus need at least six digits of precision

Improvements to the quantum algorithms:

- Estimates for an example molecule: Fe_2S_2 with 118 spin-orbitals

Gate count	10^{18}
Parallel circuit depth	10^{17}
Run time @ 10ns gate time	30 years

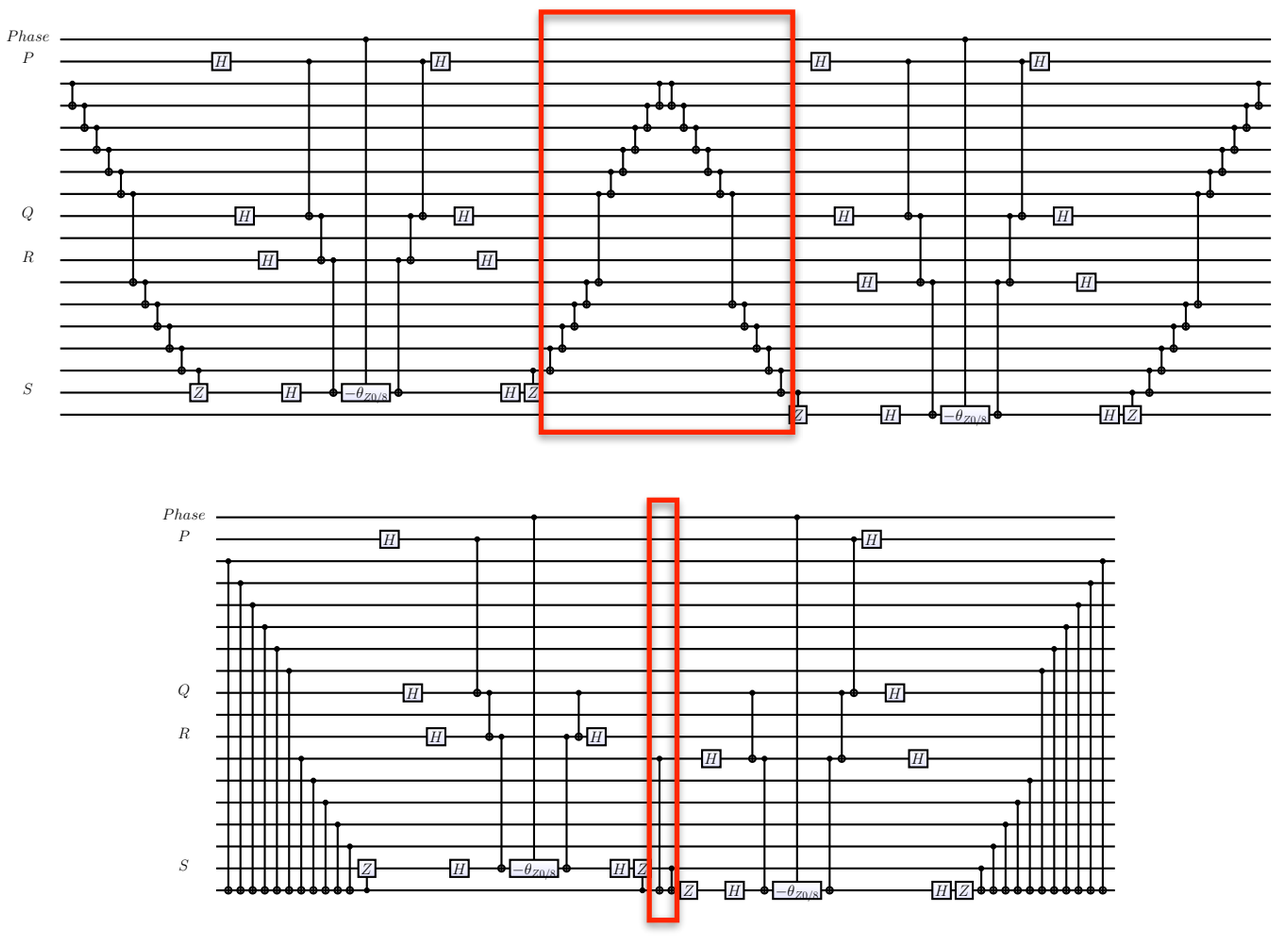
New gate count	10^{11}
Parallel circuit depth	10^{10}
Run time @ 10ns gate time	2 minutes

- Attempting to reduce the horrendous runtime estimates we achieved
  Wecker *et al.*, PRA (2014), Hastings *et al.*, QIC (2014), Poulin *et al.*, QIC (2014)
  - Cancelling of Jordan-Wigner strings: O(*N*) reduction in gates
  - Nesting of terms: O(*N*) reduction in circuit depth
  - Optimizing circuits: 4x reduction in gates
  - Smart interleaving of terms: 10x reduction in Trotter steps
  - Multi-resolution Trotter: 10x reduction in gates
  - Better quantum phase estimation: 4x reduction in rotation gates

Optimization 1: reducing Jordan-Wigner strings

M.B. Hastings *et* al., arXiv:1403.1539

- Rearrange the circuits and use an optimized ordering of terms to cancel most of the Jordan-Wigner strings between terms

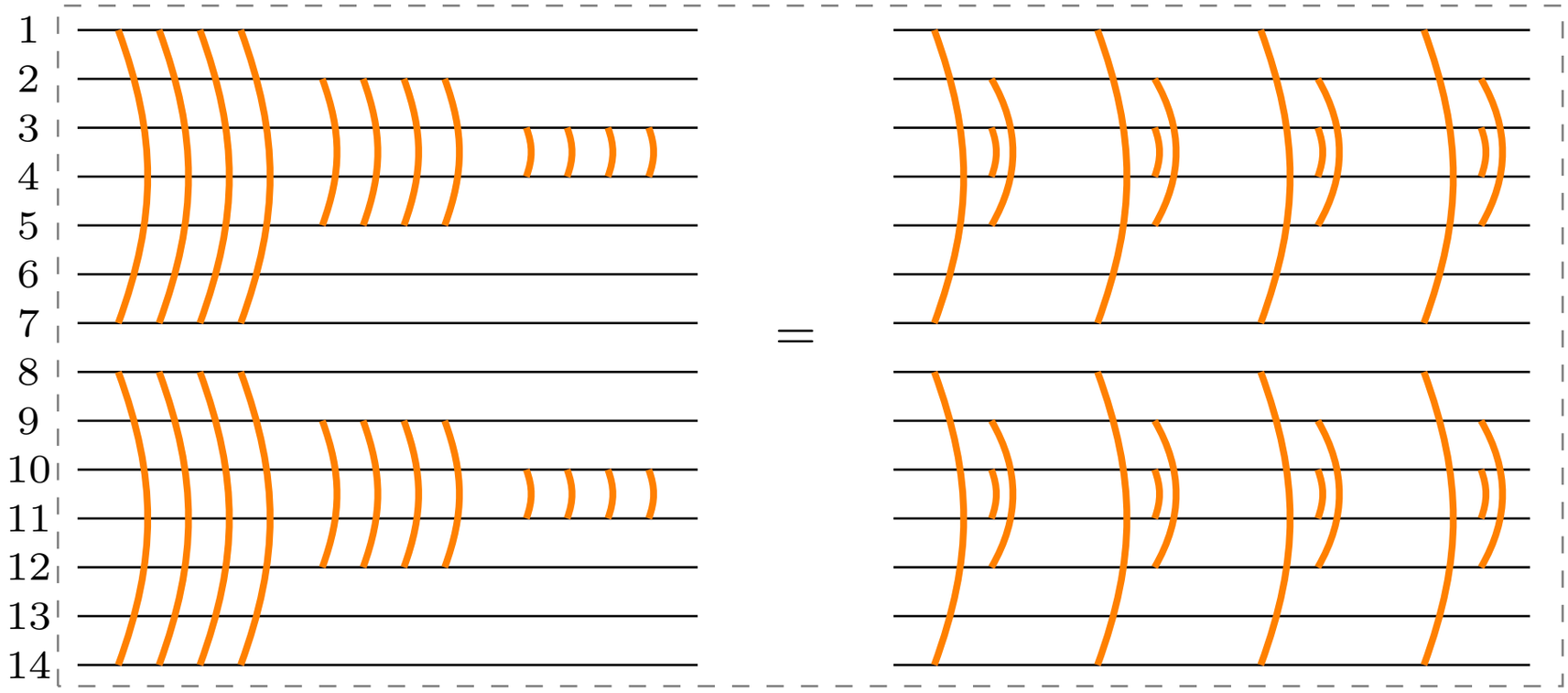


- Reduces the cost of Jordan-Wigner strings from O(*N*) to amortized O(1)

Optimization 2: Nesting of terms

M.B. Hastings *et* al., arXiv:1403.1539

- Interleave terms that seem to interfere at first sight due to overlapping Jordan-Wigner strings



- Can do O(*N*) terms in parallel for another power reduction

Optimization 3: faster phase estimation

- **Standard phase estimation**
  - propagates by time *t*
  - controlled rotation gates to implement evolution (need two normal rotations)

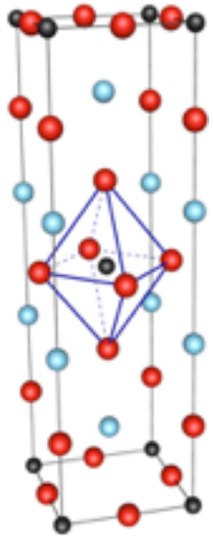
$$\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)|\phi_n\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|0\rangle|\phi_n\rangle+|1\rangle e^{-iHt}|\phi_n\rangle\right)=\frac{1}{\sqrt{2}}\left(|0\rangle+e^{-i\phi}|1\rangle\right)|\phi_n\rangle$$

- **Improved phase estimation**
  - propagates by time *t/2*
  - no controlled rotations are needed
  - 2x fewer gates, 4x fewer rotations

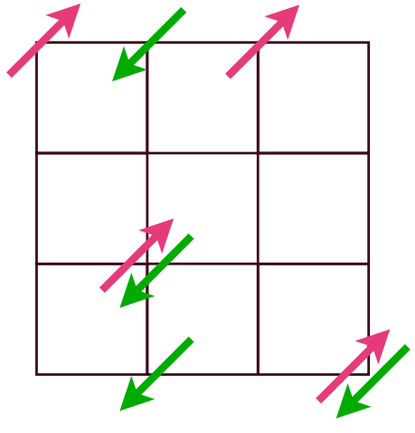
$$\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)|\phi_n\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|0\rangle e^{+iHt/2}|\phi_n\rangle+|1\rangle e^{-iHt/2}|\phi_n\rangle\right)=\frac{1}{\sqrt{2}}\left(e^{+i\phi/2}|0\rangle+e^{-i\phi/2}|1\rangle\right)|\phi_n\rangle$$

What about a room temperature superconductor?

	Full material	Hubbard model
Bands per unit cell	≈ 50	1
Unit cells needed	20x20	20x20
Number of spin-orbitals	$N \approx 80'000$	$N \approx 800$
Number of interaction terms	N^4	$O(N)$
Cirucit depth scaling	$O(N^{5.5})$	$O(1)$
Estimated runtime @ 10ns gate time	age of the universe	seconds



3D crystal structure



Hubbard model

Previous work on the Hubbard model

- Abrams and Lloyd, PRL (1997) suggested to use quantum computers for the time evolution under the Hubbard Hamiltonian
- Ortiz *et al*, PRA (2001) provided details on how to map fermions to qubits and how to measure some observables
- These seminal papers do not yet address some important parts
  - how to prepare a good trial wave function
  - mapping the time evolution onto actual quantum gates
  - estimating the circuit depth (gate count)

Direct measurements

- After preparing the ground state we can measure any desired quantity
- However, every measurement only gives a single bit!

$$\Delta O = \sqrt{\frac{\mathrm{Var} O}{M}} \Rightarrow M = O\left(\frac{1}{\epsilon^2}\right)$$ measurements are needed

Nondestructive measurements (approach I)

Wecker, Hastings *et al*, arXiv:1506.05135

- Make use of the fact that the ground state is an eigenstate of the Hamiltonian to perform non-destructive measurements

- Measurements using Hellman-Feynman theorem

$$\frac{dE_{GS}(\lambda)}{d\lambda} = \langle \Psi_{GS}(\lambda) | \frac{dH(\lambda)}{d\lambda} | \Psi_{GS}(\lambda) \rangle$$

- Add the observable to be measured as a perturbation $H(\lambda) = H + \lambda O$

- Adiabatically evolve the wave function $|\Psi_{GS}(0)\rangle \rightarrow |\Psi_{GS}(\epsilon)\rangle \rightarrow |\Psi_{GS}(-\epsilon)\rangle$

- Measure the energy and calculate the difference $\langle \Psi_{GS} | O | \Psi_{GS} \rangle \approx \frac{E_{GS}(\epsilon) - E_{GS}(-\epsilon)}{2\epsilon}$

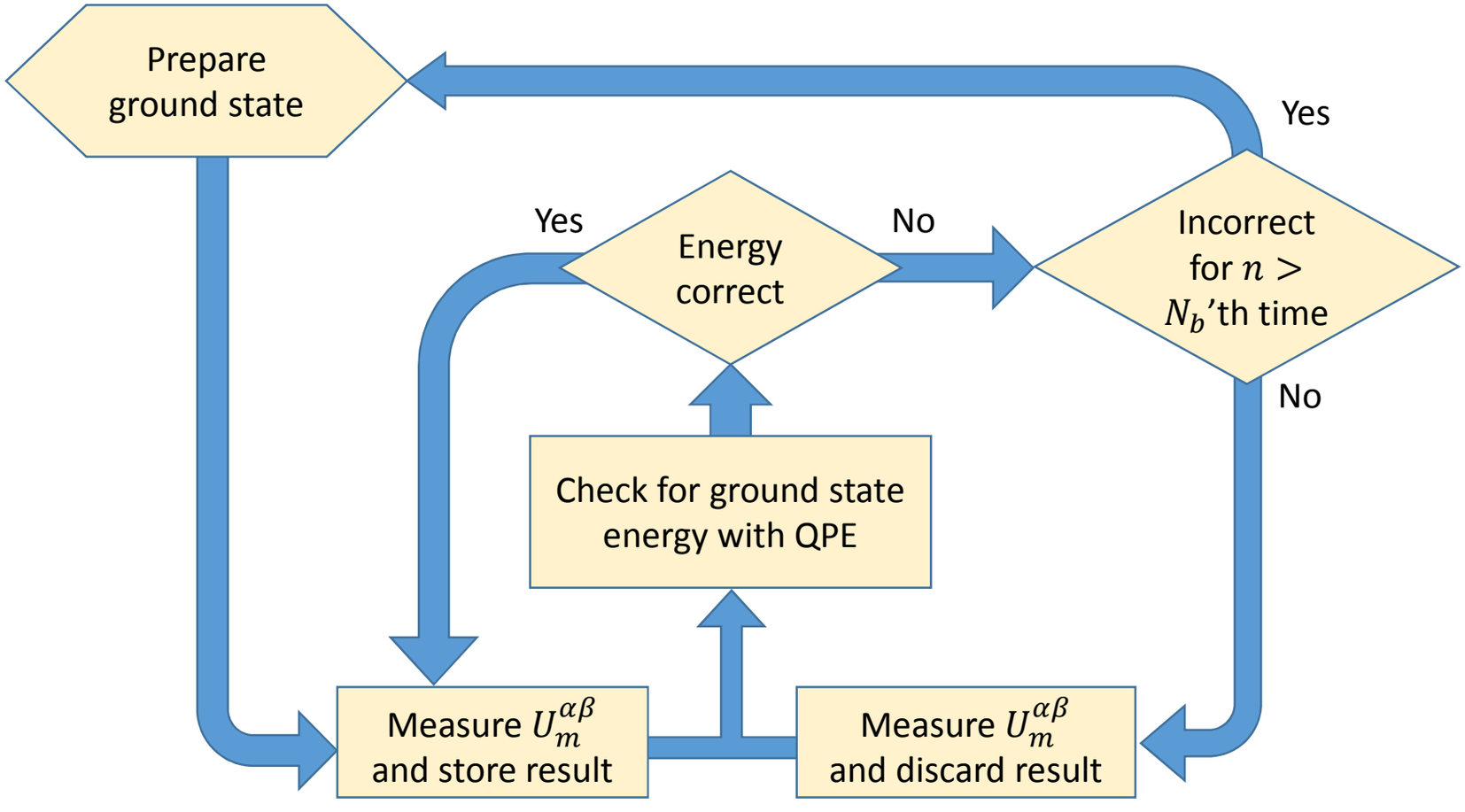
- Non-destructive and only $O\left(\frac{\log \epsilon}{\epsilon}\right)$ measurements are needed

Nondestructive measurements (approach II)

Wecker, Hastings *et al*, arXiv:1506.05135

- Recover the ground state (GS) after a destructive measurement

Efficient if we measure only a single bit
requires time $O(1/\epsilon)$ if performed coherently



From the Hubbard model to materials

- Full *ab-initio* simulation of a correlated material is too complex even on quantum hardware
- The Hubbard model is too simple
- **Solution: a hybrid approach using DMFT and quantum computers**