Lecture 4

Quantum algorithms beyond the circuit model

Quantum optimization - Quantum simulation

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Quantum algorithms beyond the circuit model

Quantum optimization - Quantum simulation

Quantum adiabatic theorem

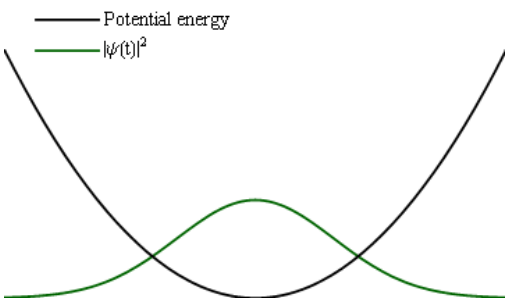
"A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum" Born-Fock (1928)

Example:
Particle in a Harmonic trap

Schrodinger equation: $$i\hbar\frac{d\psi(t)}{dt} = H(t)\psi(t)$$

Instantaneous eigenstates: $$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$

Initial condition: $$\psi(t=0) = \psi_{n_0}$$



If evolution time **slow enough** (condition, see later) $\psi(t) \approx e^{i\theta(t)}\psi_{n_0}(t)$

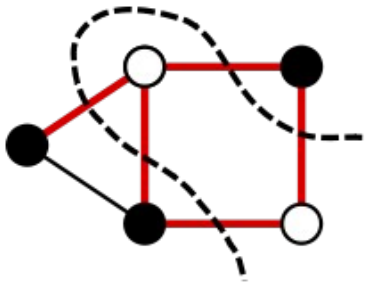
https://ocw.mit.edu/courses/physics/8-06-quantum-physics-iii-spring-2018/lecture-notes/MIT8_06S18ch6.pdf

Quantum annealing (B. Apolloni, N. Cesa Bianchi and D. De Falco (1988)

Basic Idea:

1) Encode the solution of a ‘hard’ computational problem as the ground state of a classical Hamiltonian
2) Prepare the ground-state physically via an adiabatic quantum machine
3) Extract the solution by a projective measurement

Example: Max-Cut

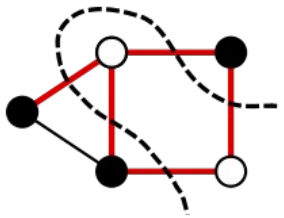


Problem:
Given a graph, divide the nodes in two parts (white versus black), such as the number of edges between the two parts is maximal

Application: Group/Market opinions analysis, micro-electronics

Complexity : NP-Hard

Quantum annealing with Max-Cut



Step 1: Encoding

Problem: Given a graph, divide the nodes in two parts (white versus black), such as the number of edges between the two parts is maximal

→ The solution is the ground-state ψ_c of a classical Ising model

$$H_C = \sum_{(i,j)\in G} \sigma_i^z \sigma_j^z$$

Step 2: Adiabatic state preparation

$$H(t) = \left(\frac{t}{\tau}\right) H_C + \left(1 - \frac{t}{\tau}\right) \sum_i \sigma_i^x$$

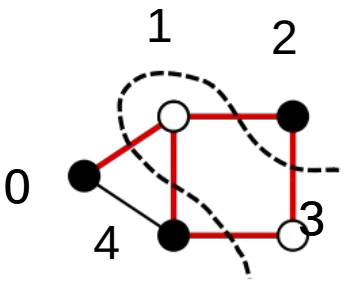
$$\psi(t=0) = |\downarrow_x, \ldots, \downarrow_x\rangle$$

$$|\downarrow_x\rangle = |\uparrow\rangle - |\downarrow\rangle$$

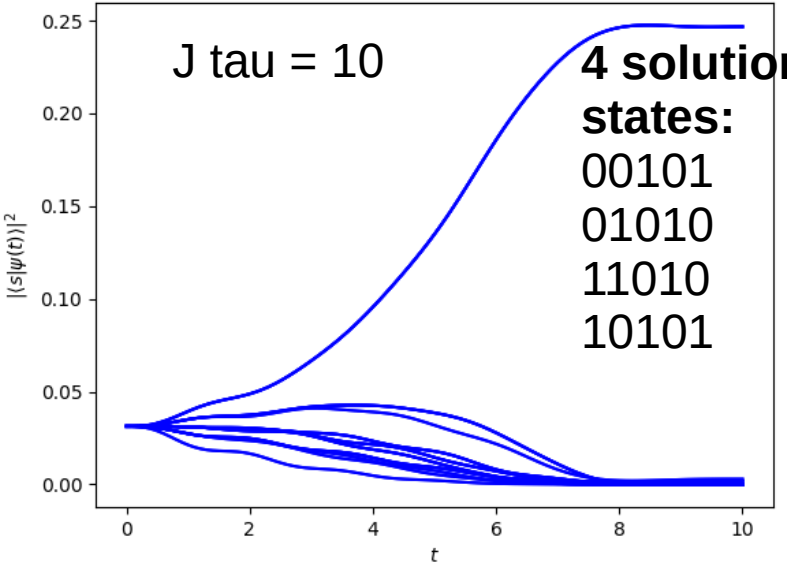
For an adiabatic ramp $\psi(\tau) \approx \psi_c$

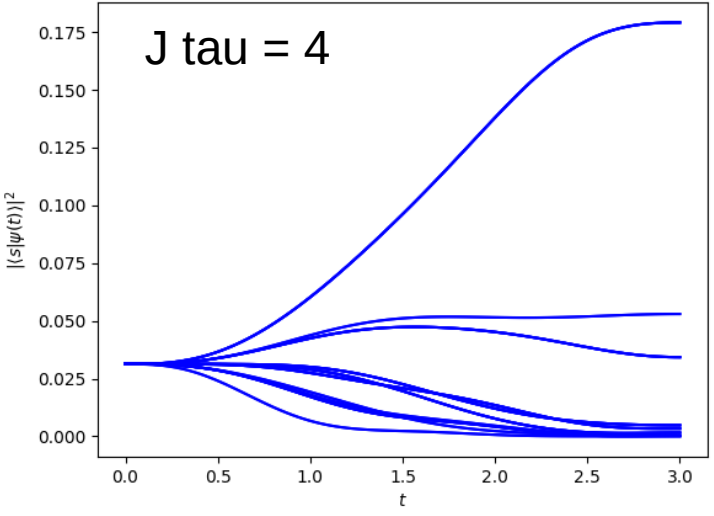
Step 3: Readout

Quantum annealing with Max-Cut



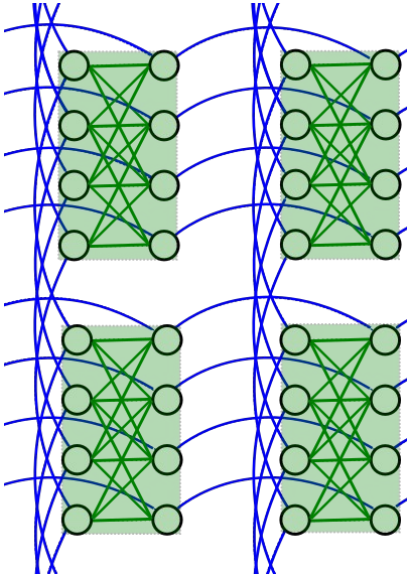
Numerical illustration (with the Python toolbox QuTip)





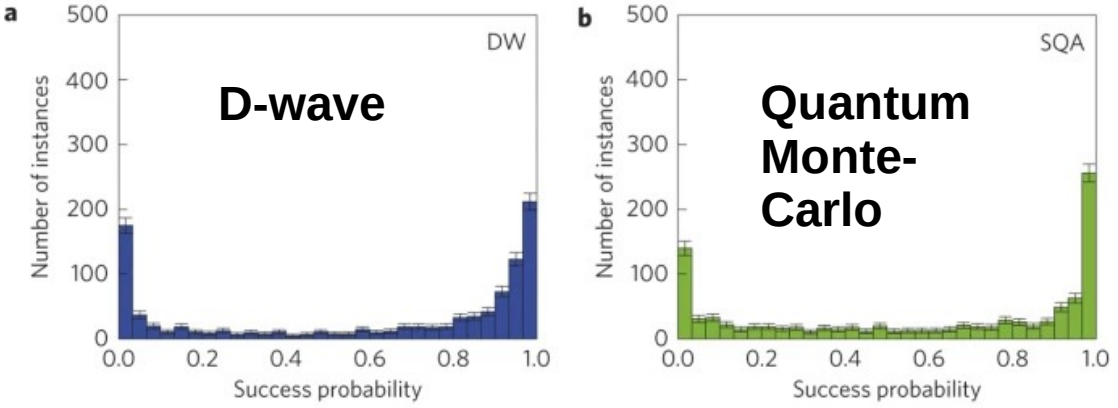
First steps towards quantum annealing

2011: D-wave quantum computing releases D-wave one with 128 qubits!



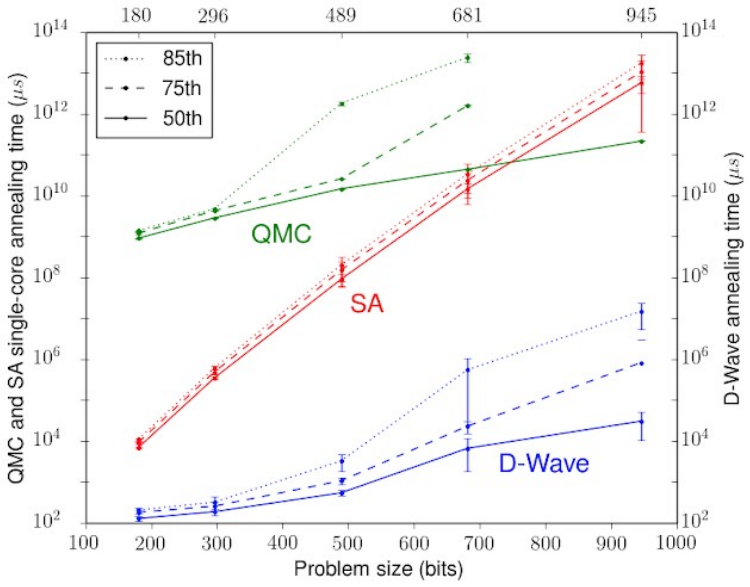
2014: Troyer and co-workers (ETH) show numerical evidence of quantum annealing with 108 qubits

But.. can also 'simulate classically' the whole process via Quantum Monte Carlo Simulations..



First steps towards quantum annealing

http://arxiv.org/abs/1512.02206 → Google responds with D-wave 2X...



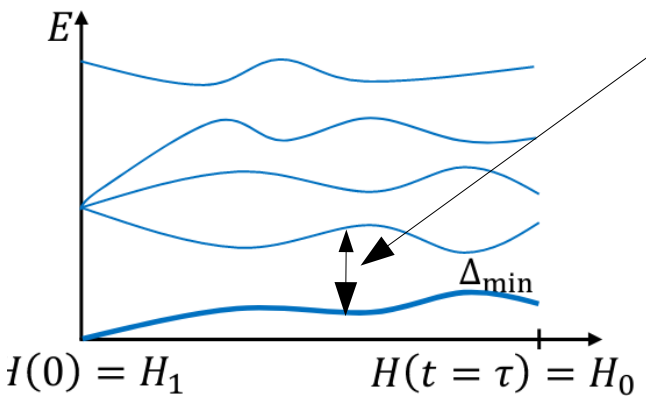
D-wave is promising, but are there **fundamental limitations...**

Limitation of quantum annealing: quantum-phase transitions

https://arxiv.org/pdf/1903.06559.pdf

Adiabatic condition for a quantum Annealer: $\tau \gg \max_{0 \le s \le 1} \frac{\left| \langle 1(s) | \frac{d\tilde{H}(s)}{ds} | 0(s) \rangle \right|}{\Delta_{1,0}(s)^2}. \quad (t = s\tau)$

Instantaneous ‘gap’



→ **Performance of quantum annealing are governed by the size of the gap’**

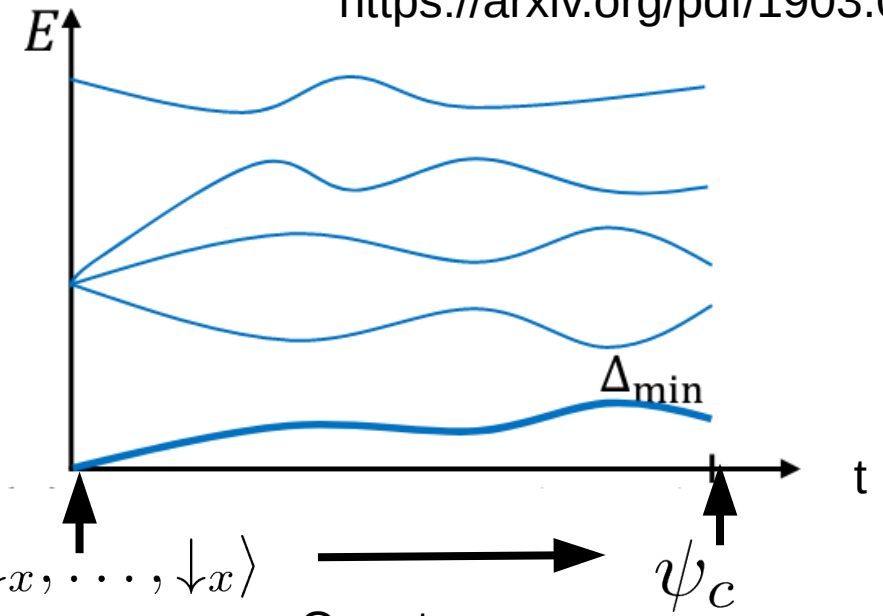
Limitation of quantum annealing: quantum-phase transitions

https://arxiv.org/pdf/1903.06559.pdf

What is the size of the gap?

(Transverse Ising Model)

$$H(t) = \left(\frac{t}{\tau}\right) H_C + \left(1 - \frac{t}{\tau}\right) \sum_i \sigma_i^x$$



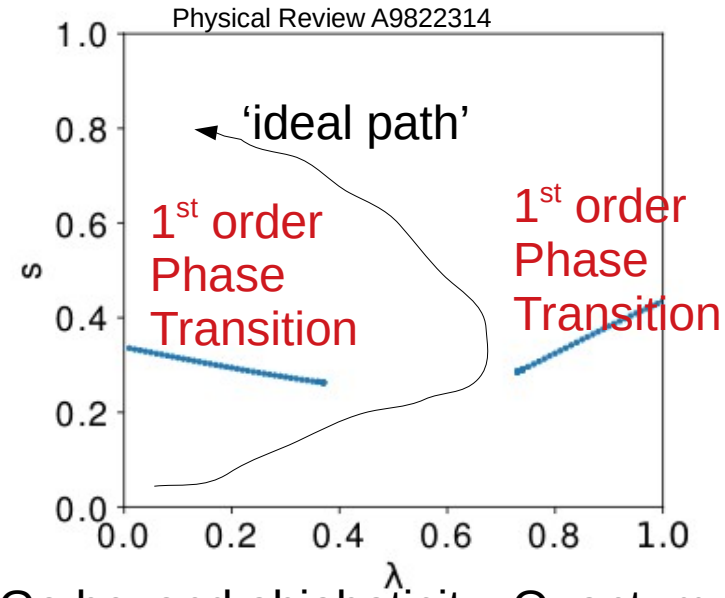
First order phase transition: gaps closes exponentially with system size → **HARD PROBLEM**

Second-order phase transition: polynomial closure → **DOABLE**

Limitation of quantum annealing: quantum-phase transitions

Current efforts:

Solution (1) Try to avoid first order phase transitions



Extra-control parameter $\rightarrow H(s, \lambda)$

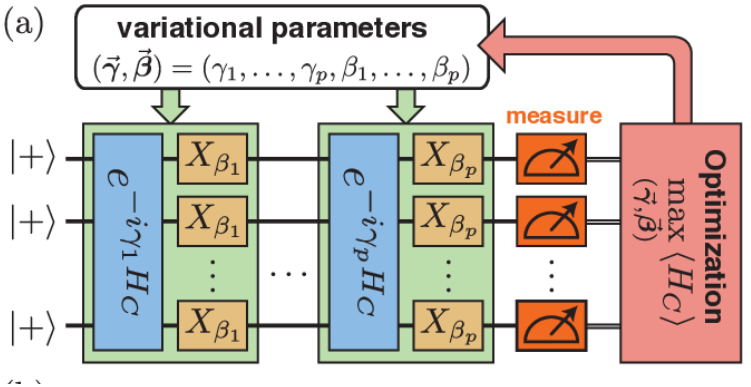
Solution (2) Go beyond abiabaticity: Quantum Approximate Optimization Algorithm (QAOA)

The quantum approximate optimization algorithm (E. Farhi 2014)

Problem (ex: Maxcut) H_C

Step 1: Build a candidate for the solution via a quantum device

$$\psi = \prod_{j=1}^{\eta} e^{i\alpha_j H_C} e^{i\beta_j \sum_l \sigma_l^x} |0000000\rangle$$

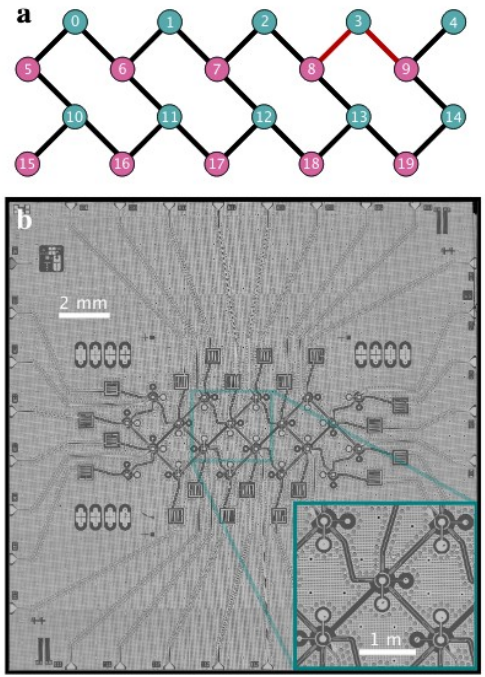


Step 2: Measure the cost-function $\langle\psi| H_c |\psi\rangle$

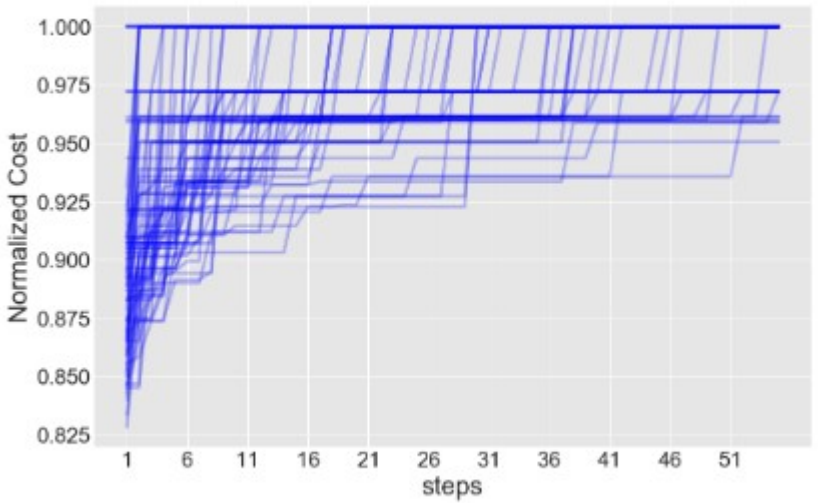
Step 3: Feed the result into a classical optimization algorithm and try **Step 1** with new parameters (α_j, β_j)

The quantum device is used for ‘fast’ evaluation of a cost function, exploring many quantum paths

The quantum approximate optimization algorithm (E. Farhi 2014)



Example: Rigetti https://arxiv.org/pdf/1712.05771.pdf



Quantum annealing → QAOA: Promising for classical problems (ex: Max-Cut)
Can we solve **quantum** problems?

Solving quantum problems with quantum computers

Nature Communications volume 5, Article number: 4213 (2014)

1) Quantum Chemistry

Goal: Find Ground-State configuration of a molecule

$$\mathcal{H}(R) = \sum_{pq} h_{pq}(R)\hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} h_{pqrs}(R)\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Electron creation operator

Single-electron orbital

$$h_{pq} = \int dr\ \chi_p(r)^* \left(-\frac{1}{2}\nabla^2 - \sum_\alpha \frac{Z_\alpha}{|r_\alpha - r|}\right) \chi_q(r) \quad (2)$$

$$h_{pqrs} = \int dr_1\ dr_2\ \frac{\chi_p(r_1)^* \chi_q(r_2)^* \chi_r(r_1)\chi_s(r_2)}{|r_1 - r_2|} \quad (3)$$

Coulomb-term

Solving quantum problems with quantum computers

Translating quantum chemistry for quantum computers

Nature Communications volume 5, Article number: 4213 (2014)

$$\mathcal{H}(R) = \sum_{pq} h_{pq}(R)\hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} h_{pqrs}(R)\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Step 1: Expression the Hamiltonian has a qubit Hamiltonian: **Jordan-Wigner Transformation**

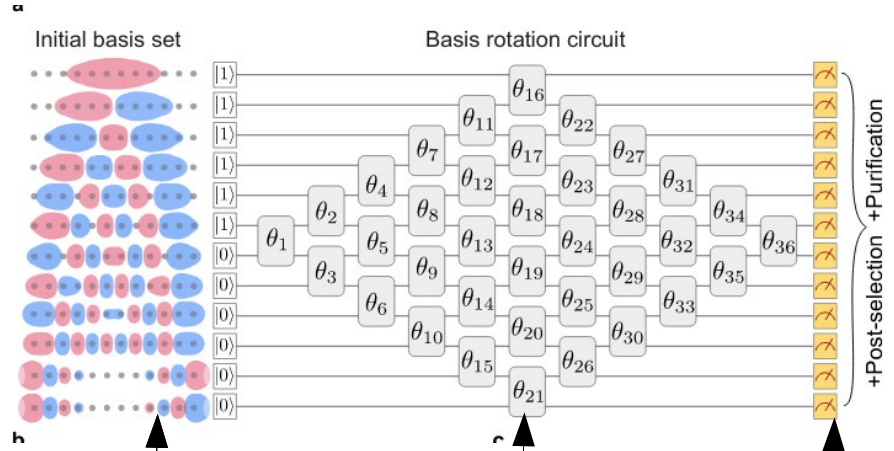
$$\hat{a}_j \rightarrow I^{\otimes j-1} \otimes \sigma_+ \otimes \sigma_z^{\otimes N-j}$$
$$\hat{a}_j^\dagger \rightarrow I^{\otimes j-1} \otimes \sigma_- \otimes \sigma_z^{\otimes N-j}$$

Step 2: Find the ground-state by quantum-approximate-optimization-algorithm (In this context, it's called **Variational Quantum Eigensolver (VQE)**

Solving quantum problems with quantum computers

Illustration with Google's Sycamore

https://arxiv.org/pdf/2004.04174.pdf

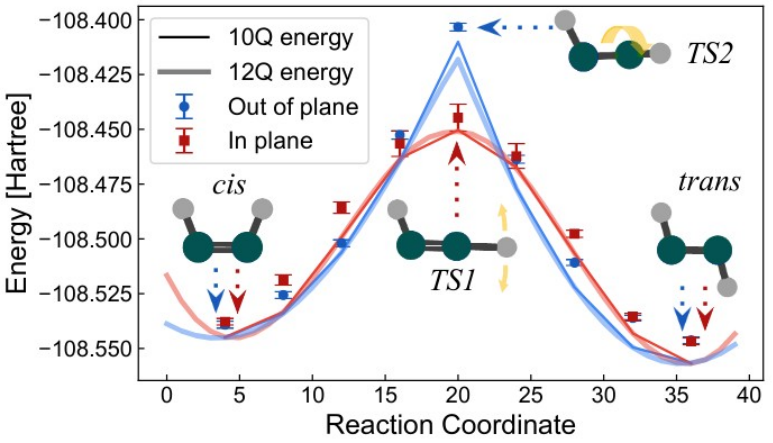


1 qubit = 1 orbital

Preparation of a ground-state candidate

Energy measurement

Repeat with different parameters



Conclusions on quantum optimization

	Quantum annealing	Quantum Approximate-Optimization Algorithm	Variational Quantum Eigensolver
Typical Problem:	Classical	Classical	Quantum
Limitations:	Scaling of the Gap	?	?

Can we solve other quantum problems?

Lecture 4

Quantum algorithms beyond the circuit model

Quantum optimization - **Quantum simulation**

Quantum Simulators

A quantum machine that could imitate any quantum system, including the physical world

Richard Feynman

Quantum Simulation: Simulation of real quantum systems by implementing the relevant Hamiltonian (in contrast to VQE)

Applications : High-Tc superconductivity, High-energy Physics, Frustrated magnetism, Topological materials, etc

Quantum Simulators

First approach: Analog quantum simulation

→ Physically realize a Hamiltonian (without a quantum computer)

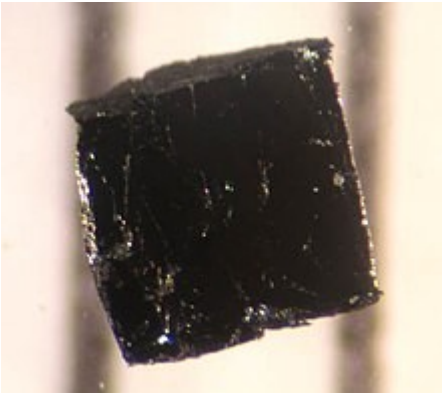
Example: Hubbard Model

$$\hat{H} = -t \sum_{i,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

- Model dynamics of valence electrons in solids

- Cannot be solved numerically in many cases

- Candidate to explain high-Tc superconductivity



Quantum Simulators

Solving the Hubbard Model via analog quantum simulation with ultra-cold atoms

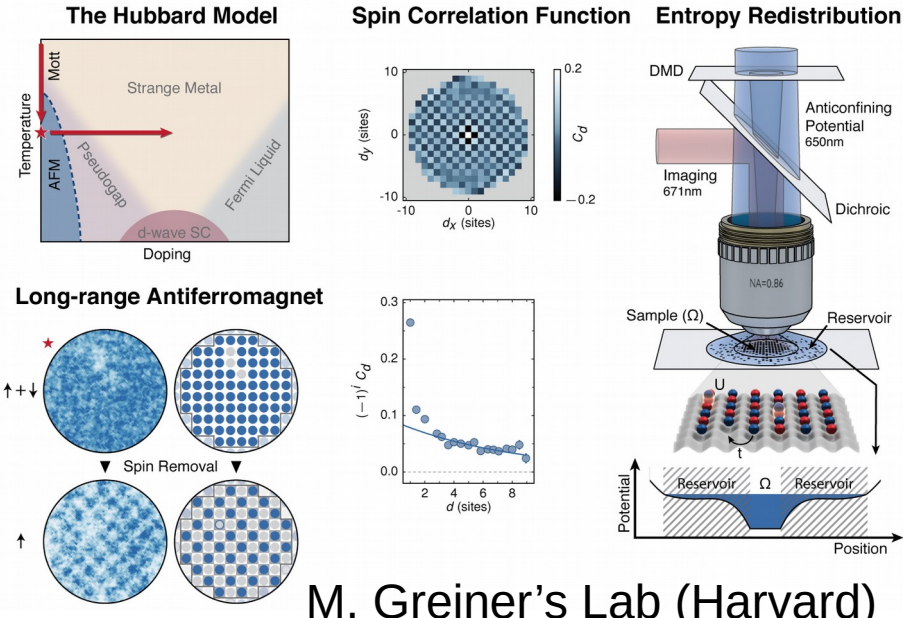
Physical Review Letters 81 (15), 3108 (1998)

$$\hat{H} = -t \sum_{i,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

Idea: Map electrons → Fermionic ultracold atoms (ex Li^6)

Laser cooling → Quantum degenerate Fermi Gas
Laser trapping → Optical lattice
Interactions → Atomic collisions
Readout → Microscope

Result match, *so far,* with theory
without need for quantum error correction



M. Greiner's Lab (Harvard)

Quantum Simulators via Quantum Computers: Digital Quantum Simulation

Step 1: Mapping to a qubit Hamiltonian H
(ex: Fermi-Hubbard → Spin via Jordan-Wigner transformation)

Step 2: 'Trotterized' time-evolution via qubit gates

$$H = \underbrace{h\sum_i \sigma_i^x}_{H_1} + \underbrace{J\sum_i \sigma_i^z\sigma_{i+1}^z}_{H_2}$$ (Transverse Ising model)

→ **Suzuki-Trotter expansion**

$$\psi(t) = e^{-iHt}\psi(0)$$

$$\psi(t) \approx \left(e^{-iH_1(t/n)}e^{-iH_2(t/n)}\right)^n \psi(0)$$

Error for a finite n (Lloyd, 1996)

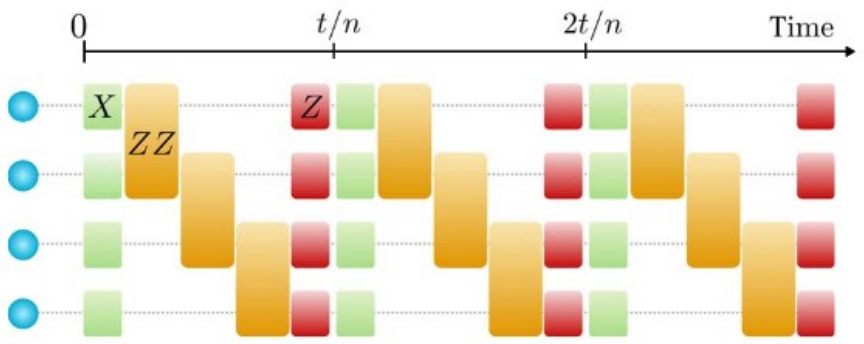
$$\mathcal{E} \sim \frac{t^2}{n}|||[H_1, H_2]|||$$

→ Requires polynomial time

Quantum Simulators via Quantum Computers: Digital Quantum Simulation

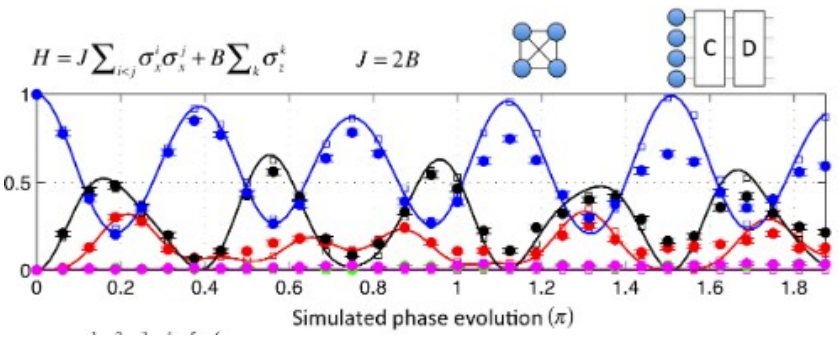
$$H = h\sum_i \sigma_i^x + J\sum_i \sigma_i^z\sigma_{i+1}^z \longrightarrow \psi(t) \approx \left(e^{-iH_1(t/n)}e^{-iH_2(t/n)}\right)^n \psi(0)$$

H_1 H_2



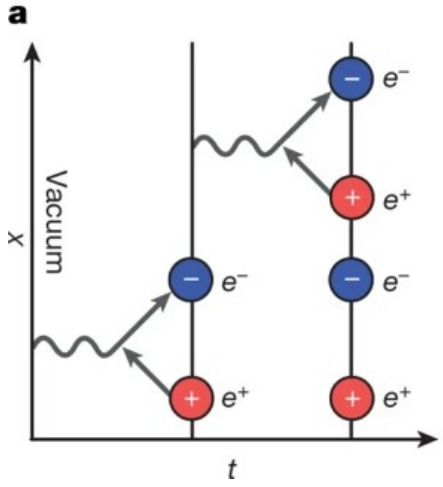
Sci. Adv.2019;5

Experimental demonstration with trapped ions (Lanyon 2011)



Quantum Simulation of high-energy physics phenomena

Illustration: Nature volume 534, pages516–519(2016)

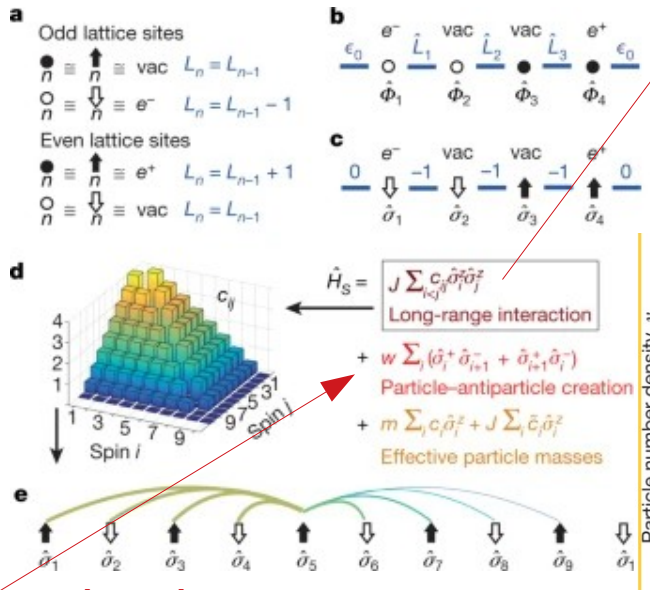


Swinger Model
(1 dimensional quantum-electro dynamics)

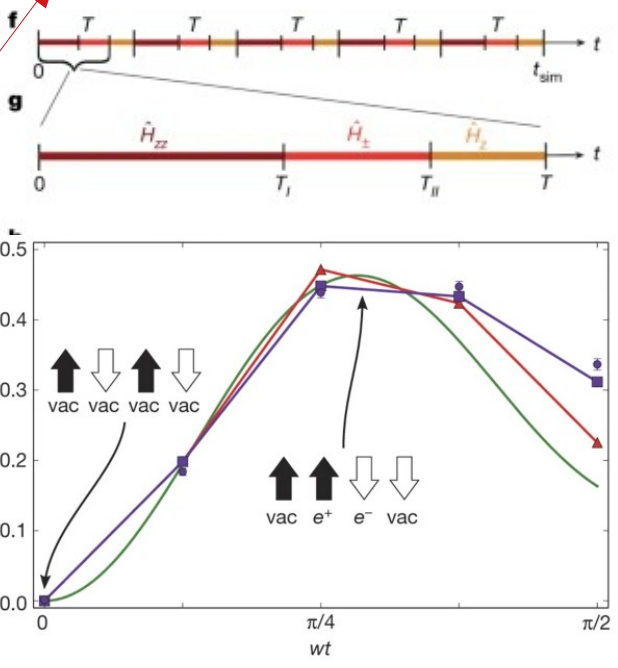
$$\hat{H}_{\mathrm{lat}} = -iw\sum_{n=1}^{N-1}[\hat{\Phi}_n^{\dagger}e^{i\hat{\theta}_n}\hat{\Phi}_{n+1} - \mathrm{h.c.}]$$
$$+ J\sum_{n=1}^{N-1}\hat{L}_n^2 + m\sum_{n=1}^{N}(-1)^n\hat{\Phi}_n^{\dagger}\hat{\Phi}_n$$

Kogut–Susskind fermions

Jordan-Wigner transformation



Digital quantum simulation



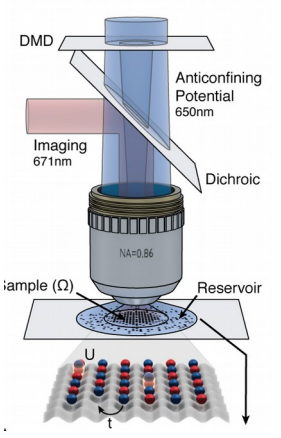
Summary: Quantum algorithms

- **Quantum computers do exist** and implement quantum circuits, following the dream of Feynman

- There are **quantum algorithms** that offer quantum speedup (Grover, Shor, etc)

- **Quantum error correction**: conceptually `solved', technical challenges

- New quantum algorithms that do not rely necessarily on quantum error correction: **Quantum optimization/Quantum simulation**



→ ***Quantum information meets many-body physics!***

A very active research field, many developments expected in the next year! (talents needed)