# Quantum algorithms

## Lecture 5: Quantum simulation/Quantum optimization

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# Outline

Quantum simulation

Quantum optimization

- Solving classical problems with quantum annealing
- Solving quantum problems

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# Introducing quantum simulation

- Feynmann original ideas related to quantum computers: 'A quantum machine that could imitate any quantum system, including the physical world'.
- Quantum simulation:
  - A synthethic quantum device, for instance a quantum computer, that mimicks a quantum system.
  - The goal is to obtain from the quantum device information about the model, beyond the possibilities of numerical simulations, and/or probe the associated physics phenomena.
  - In terms of an algorithm, the input is an Hamiltonian $H$, the output is the solution $|\psi\rangle$ of the Schrödinger equation $id\,|\psi\rangle\,/dt = H\,|\psi\rangle$, which is $|\psi\rangle = \exp(-iHt)\,|\psi\rangle$.

# Introducing quantum simulation

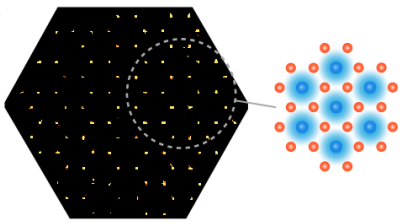
- In first approximation, there are two types of quantum systems:
  - Fermionic/bosonic models: condensed matter systems (high-TC superconductivity, impurity physics, disorder, fractional quantum Hall), high-energy physics (eg cavity quantum electrodynamics, black holes).
  - Spin models: relevant to study magnetism, quantum phase transitions, black holes.

# Introducing quantum simulation

- Example 1: The transverse Ising model

$$H = \sum_{i<j} J_{i,j} Z_i Z_j + g \sum_i X_i \qquad (1)$$

- Very rich phase diagram, relevant in particular for frustrated quantum magnetism, quantum phase transitions, etc.
- Eg Ising model on the triangular lattice (A. Browaeys's lab `https://arxiv.org/pdf/2106.15530.pdf`)



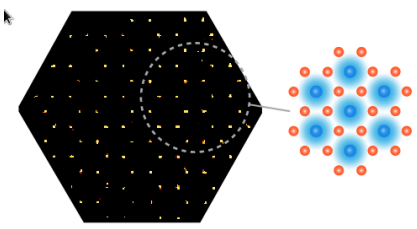
# Analog quantum simulation

- In analog quantum simulation, one realizes the model Hamiltonian

$$H = \sum_{i<j} J_{i,j} Z_i Z_j + \sum_i g X_i$$

with spin particles implemented in the quantum machine.

- Example with cold atoms:
  - For each atom $i$, identify two electronic levels $|0\rangle$, $|1\rangle$.
  - $J_{i,j} Z_i Z_j$ represents dipolar interactions
  - $g X_i$ is a laser-driven electronic coupling.



# Digital quantum simulation

- In digital quantum simulation, one 'programs' the model with a quantum computer
- The goal is to simulate the Schrödinger equation, we need to implement the quantum circuit $U(t) = e^{-iHt}$ with a universal set of gates.

$$H = \sum_{i<j} J_{i,j} Z_i Z_j + \sum_i g X_i$$

- Lloyd (1996): digital quantum simulation can be efficiently implemented in a quantum computer, i.e, with a number of gates that scales polynomially with the number of qubits and time.

# Digital quantum simulation

- Starting point to implement our circuit: Suzuki-Trotter decomposition

$$e^{-i(H_1+H_2)t} = \lim_{m\to\infty} \left(e^{-iH_1 t/m} e^{-iH_2 t/m}\right)^m$$

- With for a fixed $m$, an error $O(t^2/m||[H_1, H_2||)$ (Lloyd, Science 1996).
- Exercice: Write the quantum circuit for a given $m$ for the quantum Ising model

$$H = \sum_{i<j} J_{i,j} Z_i Z_j + \sum_i g X_i$$

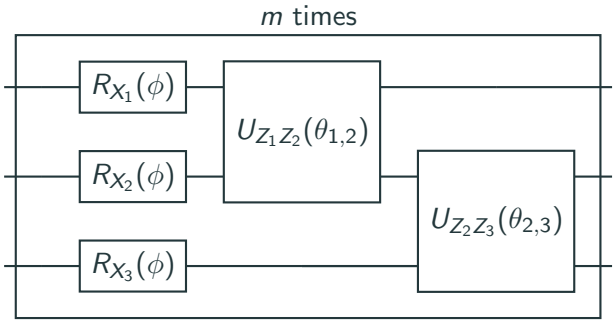
# Digital quantum simulation of the transverse Ising model

- $$e^{-iHt} \approx \left( \prod_{i<j} U_{Z_i Z_j}(\theta_{i,j}) \prod_i R_{X_i}(\phi) \right)^m \tag{2}$$

  with $U_{Z_i Z_j}(\theta_{i,j}) = e^{-i\theta_{i,j}(Z_i \otimes Z_j)/2}$, $\theta_{i,j} = 2J_{i,j}t/m$, $R_{X_i}(\phi) = e^{-i\phi X_i/2}$ and $\phi = 2gt/m$.
- where we have used that, for commuting operators $A, B$, $e^{A+B} = e^A e^B$

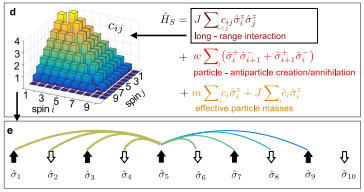
# Digital quantum simulation

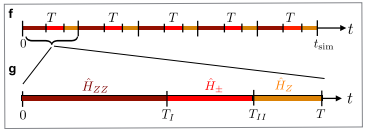
- Example with three qubits, 1D nearest neighbor couplings:



# Digital quantum simulation

- Various implementations over the last years with trapped ions and superconducting qubits
- Example for cavity quantum electrodynamics (Martinez et al, Nature 2016 )




- Can we use analog/digital quantum simulation to prepare ground states, i.e $|\psi^{(0)}\rangle$ such that ?

$$H |\psi^{(0)}\rangle = E^{(0)} |\psi^{(0)}\rangle \tag{3}$$

with the smallest possible $E^{(0)}$.

# Outline

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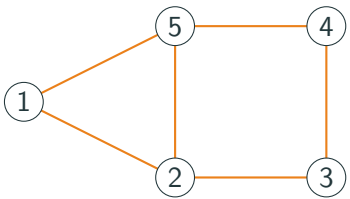
# Quantum optimization

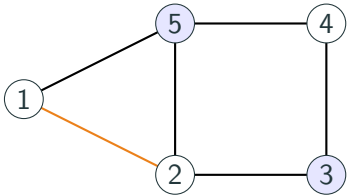
- Quantum optimization aims at finding the groundstate $|\psi^{(0)}\rangle$ of a 'problem' Hamiltonian $H^{(0)}$.
- The problem Hamiltonian can encode
  - A classical problem (hard classical optimization problem)
  - A quantum problem (physics model, quantum chemistry)
- Let us first describe the full strategy for trying to solve classical problems with quantum computers.

# Hamiltonian encoding of classical problems

- Let us consider the NP-complete problem Max-Cut as example.
- Let $G$ be a graph of $n$ nodes with arbitrary connectivity $J_{i,j} = 0, 1$
- Let us label the possible bi-partitions of this graph in terms of $2^n$ bitstrings $x_1, \ldots, x_n$ [The 'state' $x_i = 0$ $(= 1)$ means $i$ belongs to the first (second respectively) partition].
- Problem: What is the maximal possible number of 'cuts', i.e the maximal numbers of pairs $(i, j)$ such that $J_{i,j} = 1$ and $x_i \neq x_j$.



- This is one optimal solution $x = (0, 0, 1, 0, 1)$, with max-cut=5.



# Hamiltonian encoding of classical problems

- Max-Cut is one of the NP-complete problems that can be mapped to a classical Hamiltonian problem
- The ground state $|\psi_p^{(0)}\rangle$ of $H_p = \sum_{i<j} J_{i,j} Z_i Z_j$ is the solution of Max-Cut, because

$$H_p |x\rangle = \left(\#_{\mathrm{couplings(J)}} - 2\#_{\mathrm{Cuts(x)}}\right) |x\rangle \tag{4}$$

- Definition: A 'classical Hamiltonian' is a Hamiltonian that is diagonal is the 'computational basis' $\{|x\rangle\}$.
- A quantum algorithm to find ground states of classical Hamiltonian: Quantum annealing

# Quantum annealing relies on the quantum adiabatic theorem

- Let $H(t) = h(t/\tau)$, a time-dependent Hamiltonian, such that $h(0) = H_e$ and $h(1) = H_p$
- If I can prepare the quantum system in the groundstate of the 'easy' Hamiltonian $|\psi(t=0)\rangle = |\psi_e^{(0)}\rangle$,
- Then it will end up approximately at time $t = \tau$ in the groundstate of the 'problem' Hamiltonian

$$|\psi(t=\tau)\rangle = |\psi_p^{(0)}\rangle \tag{5}$$

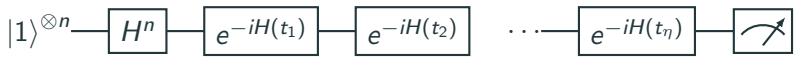
provided the adiabatic condition (see eg Messiah's book on quantum mechanics)

$$\tau \gg \max_{s\in[0,1]} \left( \frac{\langle \psi^{(0)}(s) | \dot{h}(s) | \psi^{(1)}(s) \rangle}{|E^{(1)}(s) - E^{(0)}(s)|^2} \right) \tag{6}$$

with $(|\psi^{(k)}(s)\rangle, E^{(k)}(s))$ the eigenstate decomposition of $h(s)$.

# Quantum annealing algorithm of Ising models

1. Encode your problem in a classical Ising Hamiltonian $H_p$ (as seen for Max-Cut)
2. Prepare the groundstate $|\psi_e^{0)}\rangle = (H|1\rangle)^{\otimes n}$ of the easy Hamiltonian $H_e = g\sum_i X_i$.
3. Evolve via analog or digital quantum simulation with $H(t) = (t/\tau)H_p + (1 - t/\tau)H_e$ and measure the answer $|x\rangle$



# Quantum annealing

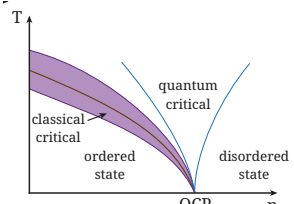
- 2011, D-wave announces the first commercial quantum computer: a quantum annealer with an analog quantum simulator made of superconducting qubits.

(wikipedia)

- But what of performances can we expect, compared with classical algorithms?

# Quantum annealing

- Adiabatic condition: Computation time $\tau$ scales as $1/\Delta^2$, with the 'minimal gap' $\Delta = \min_s[E^{(1)}(s) - E^{(0)}(s)]$.
- Going from an easy Hamiltonian $H_e = \sum_i X_i$ to a problem Hamiltonian $H_p = \sum_{i,j} J_{i,j}$, the qubits change macroscopically their configurations, a phenomenon studied in condensed matter as quantum phase transitions.




(wikipedia)

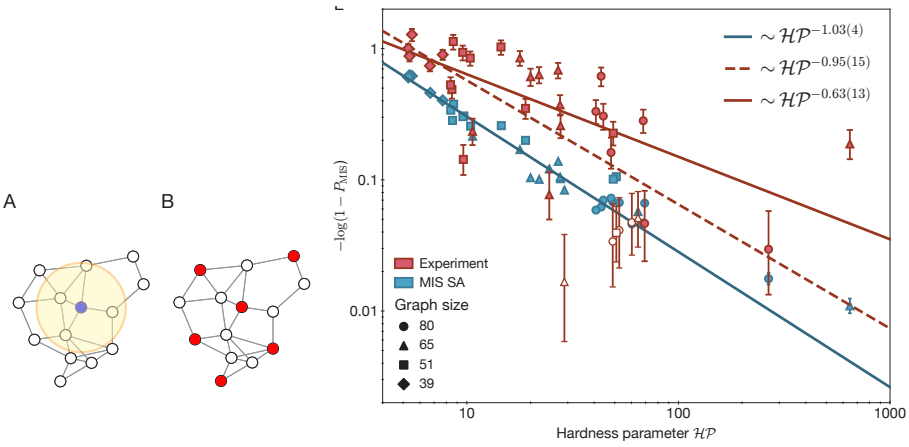
- The scaling of the gap with the problem size, the qubit number $n$, depends on the nature of a quantum phase transition

# Quantum speedup with Rydberg atoms

- Farhi et al (arxiv:0201031.pdf): There are problems that require a polynomial runtime with an adiabatic quantum computer, and that would require an exponential time with simulated annealing (a classical algorithm of reference for optimization problems).
- Troyer et al (Nature Physics 2014) quantum Monte carlo methods that simulate the quantum annealing circuit with a classical computer.
- The question of quantum annealing being able to outperform all classical methods is an open question.

# How does the gap scale?

Recent experiment with Rydberg atoms: observation of quantum speedup w.r.t simulated annealing (arxiv:2202.09372, Science 2022)



# Solving quantum problems

- Maybe it's easier to obtain quantum speedup for quantum problems?
- Quantum chemistry: Consider a molecule of $B$ with $b = 1 \dots B$ electrons. In the Born-Oppenheimer, the nuclear coordinates $\mathcal{R} = (\vec{R}_a)$, $a = 1 \dots A$ are 'frozen' and we are looking for the groundstate of the electronic Hamiltonian

$$\mathcal{H}(\mathcal{R}) = \sum_{b=1}^{J} \left( -\frac{1}{2}\nabla_b^2 + \sum_{a=1}^{A} \frac{Z_i z_j}{|\vec{R}_a - \vec{r}_b|} \right) + \sum_{b<b'} \frac{z_b z_{b'}}{|\vec{r}_b - \vec{r}_{b'}|} \tag{7}$$

# Second quantization approach to quantum chemistry

- The quantum chemistry Hamiltonian is expressed in a finite basis of $n$ single electron orbitals $\phi_i(\vec{r})$
- We obtain the second quantized Hamiltonian

$$H(\mathcal{R}) = \sum_{i,j} h_{i,j} a_i^\dagger a_j + \sum_{i,j} h_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l \tag{8}$$

  where the fermionic operator $a_i^\dagger$ creates an electron in the orbital $i$.
- The tensor $h_{i,j}$, $h_{i,j,k,l}$ are one electron, two-electron orbital integrals that can be calculated classically easily (e.g Google's OpenFermion library)

# From electrons to qubits

$$H(\mathcal{R}) = \sum_{i,j} h_{i,j} a_i^\dagger a_j + \sum_{i,j} h_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l \tag{9}$$

- The fermionic operators satisfy anti-commutation relations

$$\{a_i^\dagger, a_j\} = \delta_{i,j}, \quad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0 \tag{10}$$

- One approach to solve quantum chemistry on a quantum computer consists in mapping fermions to qubits

# From electrons to qubits

- Jordan-Wigner transformation (Exercices 5): I can encode $n$ fermionic orbitals on $n$ qubits via the transformation

$$a_i = (\prod_{j=1}^{i-1} Z_j)\sigma_i \tag{11}$$

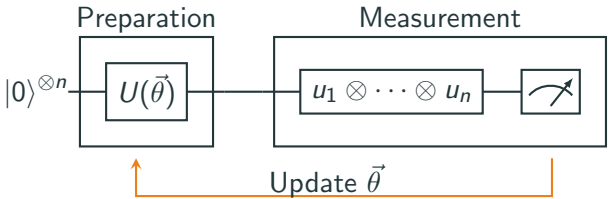
  with $\sigma_i = |0\rangle_i \langle 1|$.
- I can find the ground state of the corresponding qubit Hamiltonian on a quantum computer using quantum optimization.

# From quantum annealing to the variational quantum eigenvolver

- I can in principle do quantum annealing on the problem Hamiltonian $H_p = H(\mathcal{R})$, but we have the same type of limitations as for solving classical problems.
- One alternative: variational quantum eigensolver (VQE), our last quantum algorithm (limitations are not yet understood...) (Peruzzo et al, Nat. Comm. 2014)

# The variational quantum eigenvolver

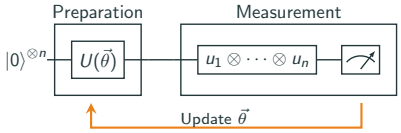
- In VQE, one performs a closed loop classical optimization of variational quantum circuits




- The choice of $U(\vec{\theta})$ is non-trivial: I need to be able to generate with few number of gates variational wavefunctions that are close to the ground state of the problem Hamiltonian $H_p$
- Variant for classical problems: QAOA (Last quantum practical)

# The variational quantum eigenvolver

Example with Gradient descent optimization




1. Prepare $|\psi(\vec{\theta})\rangle = U(\vec{\theta})\,|0\rangle^{\otimes n}$ and measure $\langle\psi(\vec{\theta})|\,|H_p|\,|\psi(\vec{\theta})\rangle$, using multiple rotations bases $u_1, u_2, \ldots$.
2. Do the same with $\vec{\theta} \to \theta + d\vec{\theta}$
3. (On the classical computer): Compute gradient of the energies $\partial\theta_i \langle\psi(\vec{\theta})|\,|H_p|\,|\psi(\vec{\theta})\rangle$ via finite difference.
4. Adjust the $\theta$ for gradient-descent. Go back to step 1 until convergence

At the moment we do not know if we can if VQE can provide a quantum speedup as the choice of $U(\vec{\theta})$ is based on heuristics: Stay tuned!

# Quantum algorithms: Summary

- Quantum computers offer new complexity classes: the factorization problem can be solved on a quantum computer with polynomial time!
- These systems are prone to errors. Achieving fault-tolerance quantum computation is a significant technological challenge that may take decades.
- A new generation of quantum algorithms for quantum optimization: Limitations/Complexity theory is not yet understood...
- Bonus lecture: Implementation of a quantum oracle for Grover's search on SAT problems, and the quantum supremacy claim by Google.