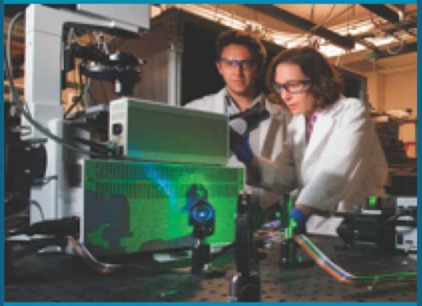
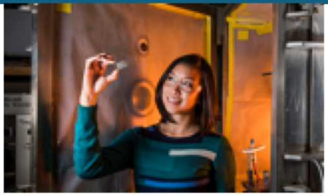
SC18 Dallas, TX | hpc inspires.

Sandia National Laboratories

SAND2019-0740C

Quantum Computing for Scientific Applications: Quantum Approaches for Discrete Optimization





PRESENTED BY

Ojas Parekh

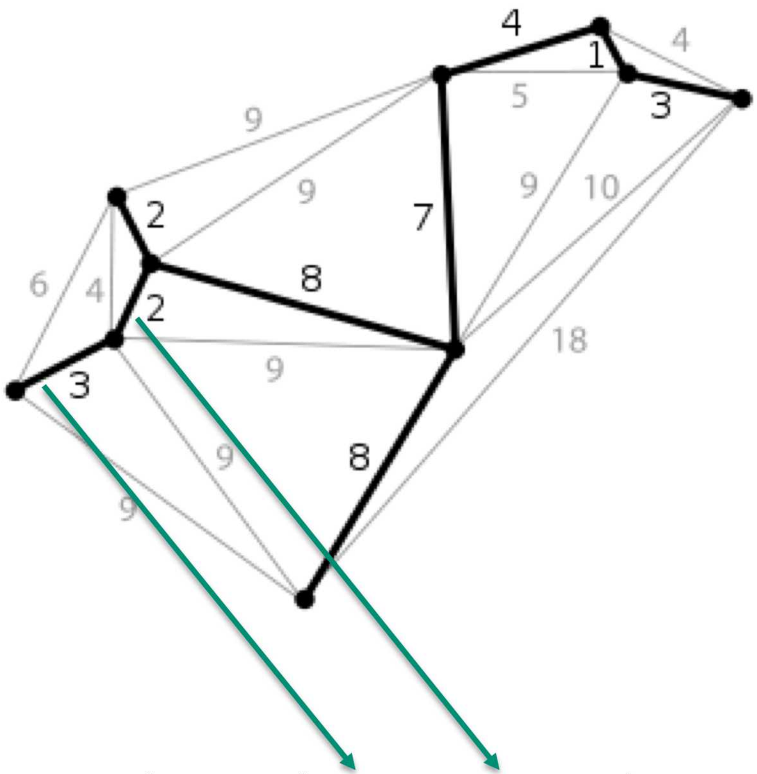
U.S. DEPARTMENT OF ENERGY | Office of Science

DOE/ASCR Quantum Algorithms Teams Program

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Discrete Optimization

Minimum Spanning Tree Problem



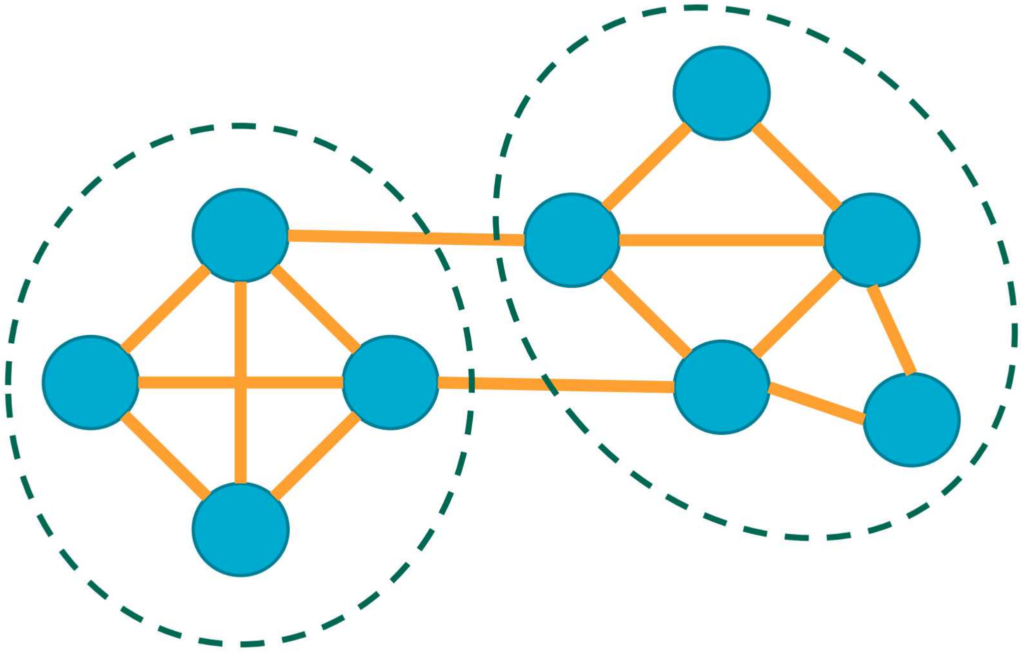
Traveling Salesperson Problem

Edge weights: (6, 3, 9, 4, 2, 9, …)
Optimal solution: (0, 1, 0, 0, 1, 0, …) binary incidence vector of solution

Scientific Computing Application: Graph Partitioning

Goal: assign computations to two processors to minimize communication

Nodes represent values to be computed, and edges represent computation dependencies



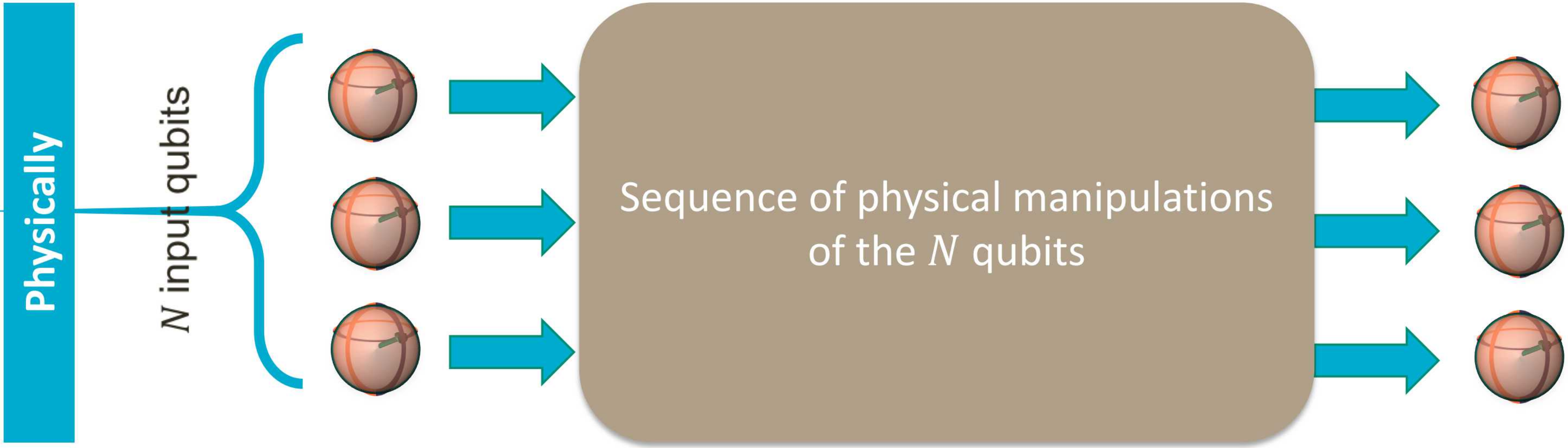
Minimum Cut: partition into two parts to minimize weight of crossing edges

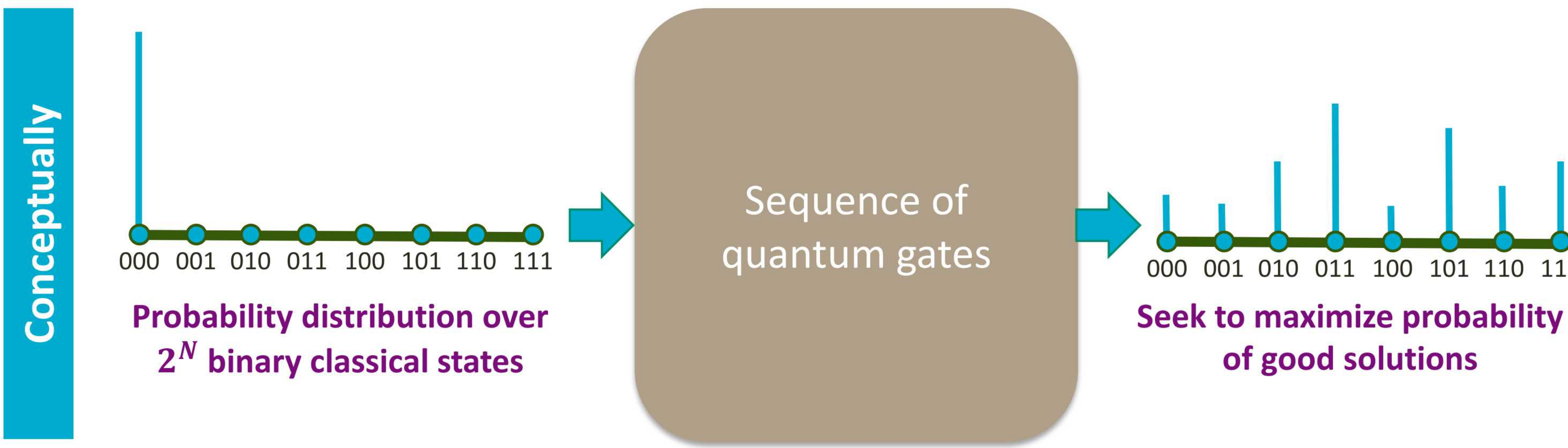
For more realistic applications, would want to:

(i) partition into *k* parts

(ii) balance load (comparable sized parts)

Quantum Algorithms Output Distributions





It's Natural to Optimize

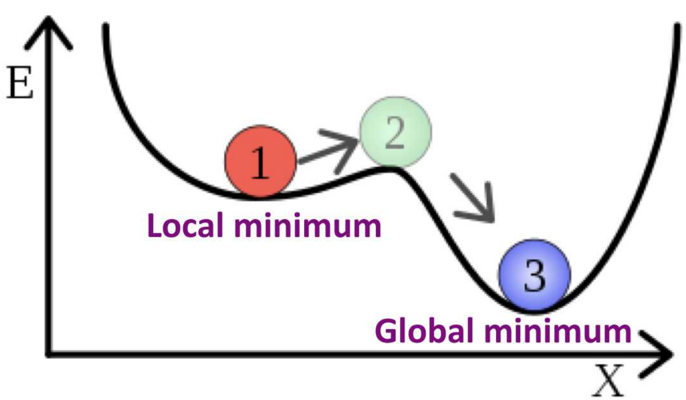
Hamiltonian eigenstate problems naturally link quantum mechanics and optimization

$$Min_{\Psi} \left\langle \psi \middle| \sum_{S} H_S \middle| \psi \right\rangle$$

Hamiltonian, $\sum_S H_S$, represents energy levels of a physical system composed of "local" parts, S

Discrete optimization problem becomes an eigenproblem on a large matrix!

Optimal discrete optimization solution ⟷ Min-energy eigenvector



Nature tends towards stable states…
So let nature solve your problems for you?

Image from https://en.wikipedia.org/wiki/Metastability

Hacking Nature to Solve Your Problems

1. Map solution values to energy levels of a physical system
2. Realize said physical system
3. Let Nature relax to a stable low-energy state

Vertices

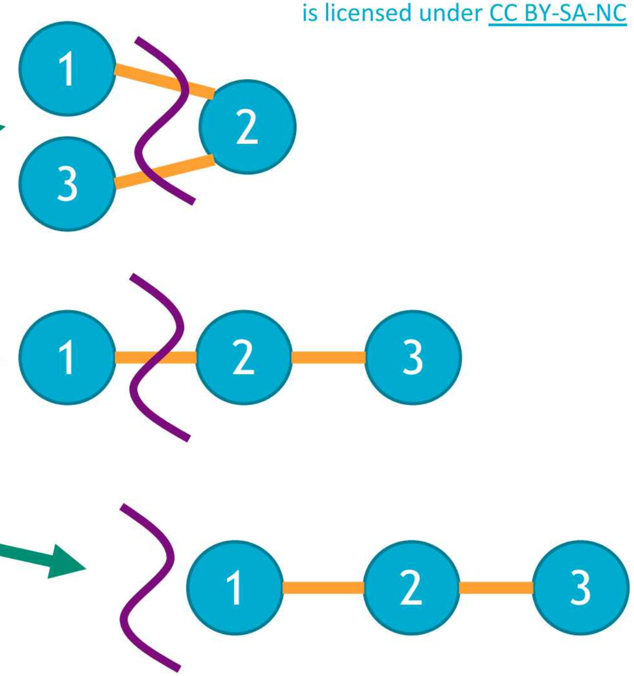
1	2	3	State
L	L	L	$\equiv \|000\rangle$
L	L	R	$\equiv \|001\rangle$
L	R	L	$\equiv \|010\rangle$
L	R	R	$\equiv \|011\rangle$
R	L	L	$\equiv \|100\rangle$
R	L	R	$\equiv \|101\rangle$
R	R	L	$\equiv \|110\rangle$
R	R	R	$\equiv \|111\rangle$

Left or **R**ight side of cut

$$
\begin{array}{cccccccc}
|000\rangle & |001\rangle & |010\rangle & |011\rangle & |100\rangle & |101\rangle & |110\rangle & |111\rangle \\
\end{array}
$$

$$
\begin{bmatrix}
0 & & & & & & & \\
 & 1 & & & & & & \\
 & & 2 & & & & & \\
 & & & 1 & & & & \\
 & & & & 1 & & & \\
 & & & & & 2 & & \\
 & & & & & & 1 & \\
 & & & & & & & 0
\end{bmatrix}
$$

Hamiltonian for cuts on a path with 3 vertices



Some cuts on a path with 3 vertices

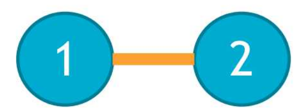
Minimum eigenstate is of form: $|\psi\rangle = \alpha|000\rangle + \beta|111\rangle$, with 0 energy

Computational Complexity Considerations

$$H = \begin{bmatrix} 0 &&&&&&& \\ & 1 &&&&&& \\ && 2 &&&&& \\ &&& 1 &&&& \\ &&&& 1 &&& \\ &&&&& 2 && \\ &&&&&& 1 & \\ &&&&&&& 0 \end{bmatrix}$$

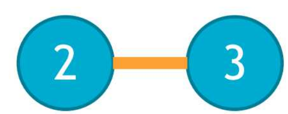
Hamiltonian is exponentially large, $2^N \times 2^N$, for an N-node graph, but it is a sum of $O(N^2)$ local 4×4 Hamiltonians, one for each edge

$$H_{12} = \begin{array}{c} \begin{bmatrix} 0 &&& \\ & 1 && \\ && 1 & \\ &&& 0 \end{bmatrix} \\ |00\rangle\ |01\rangle\ |10\rangle\ |11\rangle \end{array} \otimes I = \begin{bmatrix} 0 &&&&&&& \\ & 0 &&&&&& \\ && 1 &&&&& \\ &&& 1 &&&& \\ &&&& 1 &&& \\ &&&&& 1 && \\ &&&&&& 0 & \\ &&&&&&& 0 \end{bmatrix} \begin{matrix} |000\rangle \\ |001\rangle \\ |010\rangle \\ |011\rangle \\ |100\rangle \\ |101\rangle \\ |110\rangle \\ |111\rangle \end{matrix}$$



+

$$H_{23} = I \otimes \begin{array}{c} \begin{bmatrix} 0 &&& \\ & 1 && \\ && 1 & \\ &&& 0 \end{bmatrix} \\ |00\rangle\ |01\rangle\ |10\rangle\ |11\rangle \end{array} = \begin{bmatrix} 0 &&&&&&& \\ & 1 &&&&&& \\ && 1 &&&&& \\ &&& 0 &&&& \\ &&&& 0 &&& \\ &&&&& 1 && \\ &&&&&& 1 & \\ &&&&&&& 0 \end{bmatrix} \begin{matrix} |000\rangle \\ |001\rangle \\ |010\rangle \\ |011\rangle \\ |100\rangle \\ |101\rangle \\ |110\rangle \\ |111\rangle \end{matrix}$$



Local Hamiltonians are efficient and require manipulating only a constant number of qubits

The Power of Quantum Computing?

Extended Church-Turing Thesis

Any "reasonable" model of computing can be *efficiently* simulated by a Turing machine

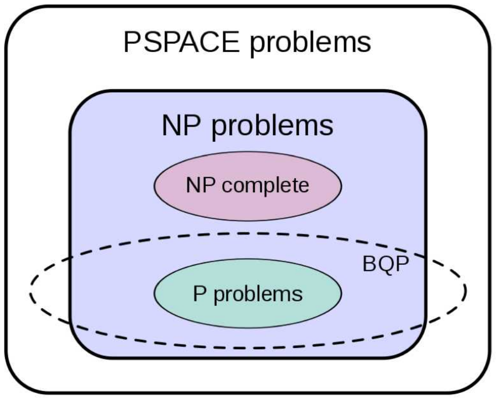


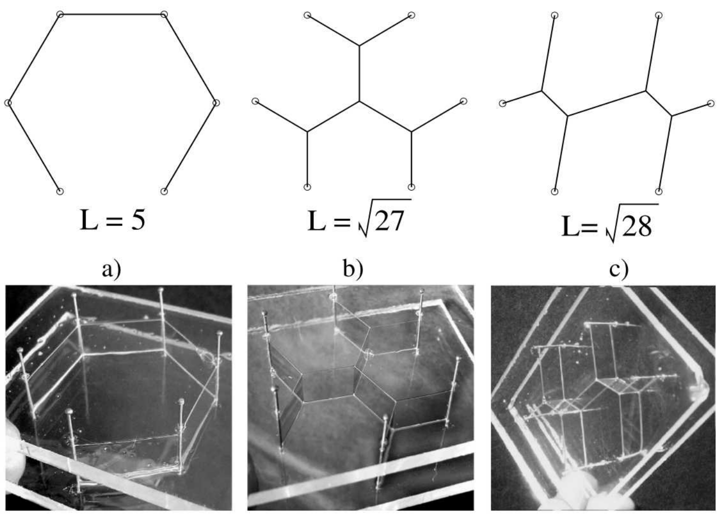
Image from https://en.wikipedia.org/wiki/BQP

It would be very surprising if quantum computers could solve NP-complete problems in quantum polynomial time (BQP).

Yet, there are problems In BQP that are very unlikely to be in classical polynomial time (P) or even NP!*

Using nature to solve optimization problems is an old idea.

In the quantum setting, it is a surprisingly powerful idea that captures universal quantum computing.



Using soap film to find Steiner Trees

[Datta, Khastgir, & Roy; arXiv 0806.1340]

*Quantum supremacy: [Preskill; arXiv 1801.00862], [Harrow & Montanaro; arXiv 1809.07442], [Aaronson & Chen; arXiv 1612.05903]

Adiabatic Quantum Computing

Explanation 1: No mathematics

1. **Confine the system in its lowest-energy configuration in a way that's easy to do.**

2. **Evolve the system in a way that keeps it in its lowest-energy configuration throughout.**

   Note: harder to do with bigger or more complex systems

3. **Read out the final state of the system; the closer the evolution was to being "adiabatic," the more probable it is that the readout is successful.**

Adiabatic Quantum Computing

Explanation 2: A bit more mathematical

1. **Confine the system in its lowest-energy configuration in a way that's easy to do.**

$$H_0 = \sum_{i=1}^{n} \sigma_x^{(i)}$$

Initial Hamiltonian

$$|\psi_0\rangle = \frac{1}{2^{n/2}} \sum_{i=1}^{2^n} |i\rangle$$

Initial ground state

2. **Evolve the system in a way that keeps it in its lowest-energy configuration throughout.**

   Note: harder to do with bigger or more complex systems

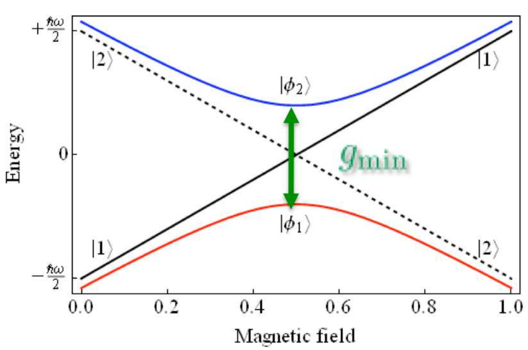
$$H(s) = (1-s)H_0 + sH_1$$

$$H_1 = h_0\, I + \sum_{i=1}^{n} h_i\, \sigma_z^{(i)} + \sum_{i,j=1}^{n} J_{ij}\, \sigma_z^{(i)} \otimes \sigma_z^{(j)}$$

Problem Hamiltonian (e.g. Cut)

3. **Read out the final state of the system; the closer the evolution was to being "adiabatic," the more probable it is that the readout is successful.**

Execution time depends on energy gap: $T \gg \frac{|\langle E_1|\dot{H}|E_0\rangle|_{\max}}{g_{\min}^2}$



Images from https://en.wikipedia.org/wiki/Adiabatic_theorem

Adiabatic Quantum Computing: [Farhi et al.; arXiv quant-ph/0001106, 2000]

The Power of Adiabatic Quantum Computing

Surprisingly, AQC is a universal model of quantum computing
(equivalent to quantum circuits within a polynomial factor resource overhead)
[Aharonov et al.; arXiv quant-ph/0405098, 2004]

Solving an optimization problem is equivalent to what any quantum computer can do!

Hamiltonian at time *s* (scaled to lie in [0,1]): $H(s) = (1-s)H_I + sH_p$
What (roughly) happens when this is applied to the current state at time *s*, $|\psi(s)\rangle$?

$$|\psi(s+\delta)\rangle = e^{-i\delta H(s)}|\psi(s)\rangle$$

[State at time $s+\delta$, assuming $H(s)$ does not change Between time s and $s+\delta$, by Schrödinger's equation]

$$= e^{-i\delta((1-s)H_I + sH_p)}|\psi(s)\rangle$$

$$\approx \underbrace{e^{-i\delta(1-s)H_I}}\underbrace{e^{-i\delta s H_p}}|\psi(s)\rangle$$

unitary operators ⟺ quantum gates

[Reasonable approximation when δ is small, By Lie-Suzuki-Trotter decomposition]

What happens if we approximate AQC by alternately applying quantum gates of the form: $e^{i\gamma H_p}$ and $e^{i\beta H_I}$?

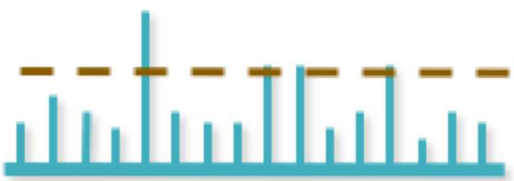
Quantum Approximate Optimization Algorithm

$$|\psi(\beta,\gamma)\rangle = \overbrace{e^{i\beta H_I}}^{\text{mixing operator}}\overbrace{e^{i\gamma H_p}}^{\text{cost operator}}|\psi_0\rangle$$

Output state depends on parameters $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$

Input state is usually easy-to-prepare ground state of $\boldsymbol{H_I}$

[Farhi et al.; arXiv:1411.4028, 2014], [Farhi et al.; arXiv:1412.6062, 2014]



$\alpha\, OPT_I$

QAOA performance is captured by expected cost:

$$\langle\psi(\beta,\gamma)|H_p|\psi(\beta,\gamma)\rangle,$$

where we seek to optimize the parameters β,γ

QAOA$_k$ applies k rounds of the mixing and cost operators:

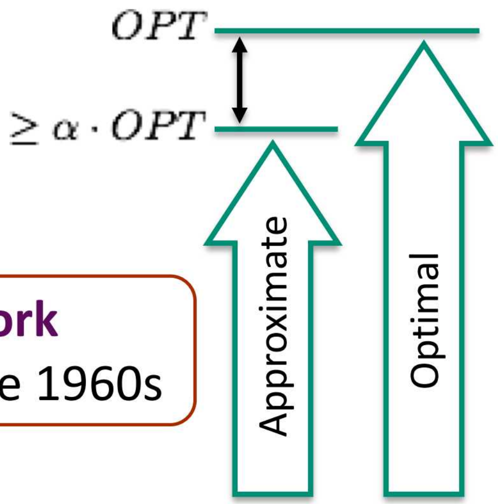
$$|\psi(\beta_1,\gamma_1,\beta_2,\gamma_2,\dots)\rangle = \underbrace{e^{i\beta_k H_I}e^{i\gamma_k H_p}}\dots\underbrace{e^{i\beta_2 H_I}\,e^{i\gamma_2 H_p}}\underbrace{e^{i\beta_1 H_I}e^{i\gamma_1 H_p}}|\psi_0\rangle$$

$\boldsymbol{k}$ iterations

This converges to an optimal solution as k grows

Why is QAOA Appealing?

- May be viewed as a discretization of Adiabatic Quantum Computing
- Results in low-depth quantum circuits, suitable for near-term quantum devices
- Generic framework for discrete optimization problems
- Can produce quantum states that are hard to sample from classically (doing something quintessentially quantum?)
  [Farhi & Harrow; arXiv:1602.07674, 2016]
- Amenable to rigorous analysis, and has outperformed best-known classical approximation algorithms for certain types of problems

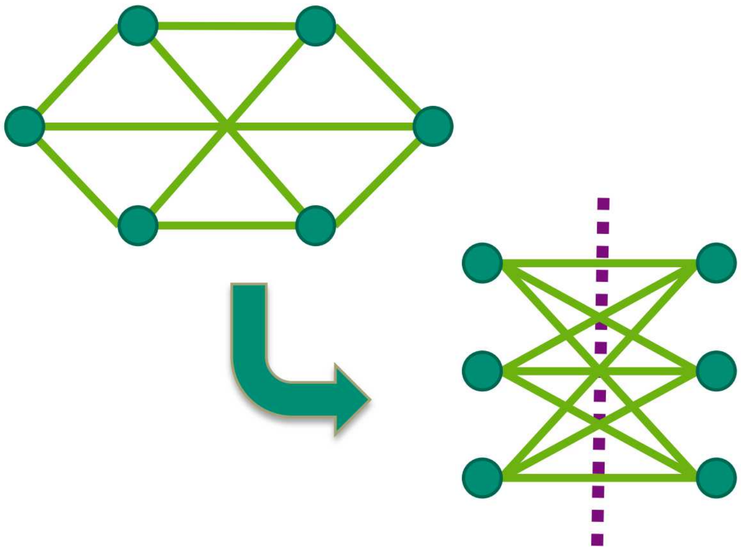


Only known quantum approximation algorithm framework
Classical approximation algorithms have been studied since the 1960s

QAOA Application: Max Cut

14

Max Cut is a fundamental NP-hard graph partitioning problem

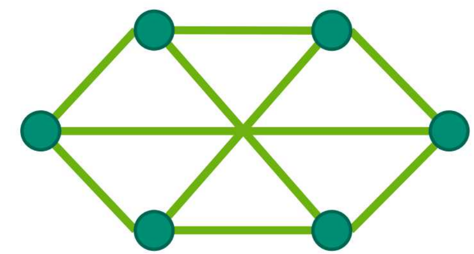


Partition vertices of a(n edge-weighted) graph two parts
to maximize (weight of) crossing edges

Quantum Outperforms Classical (…For Now)

QAOA outperforms best classical algorithm for the Max Cut problem on regular triangle-free graphs (NP-hard special case)

Researchers	Year	# Edges guaranteed	Type
Shearer	1992	$\left(\frac{1}{2}+\frac{0.177}{\sqrt{d}}\right)m$	Classical
Hirvonen, Rybicki, Schmid, Suomela	2014	$\left(\frac{1}{2}+\frac{0.281}{\sqrt{d}}\right)m$	Classical
Parekh, Ryan-Anderson Wang, Hadfield, Jiang, Rieffel	2017	$\left(\frac{1}{2}+\frac{0.303}{\sqrt{d}}\right)m$	Quantum



***m* = # edges**
***d* = # edges per vertex**

Rigorous performance proof: Only known quantum approximation algorithm outperforming the best-known classical algorithm

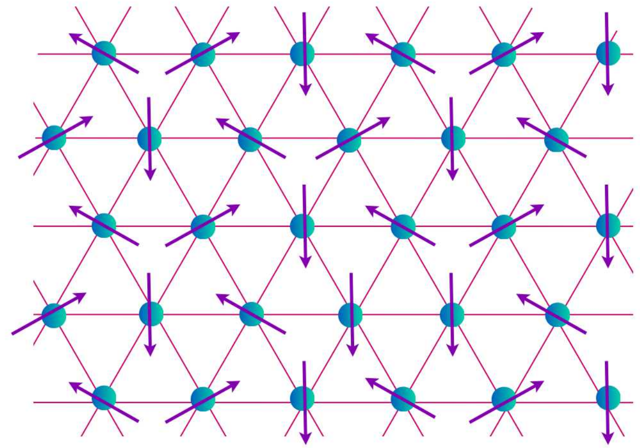
Discrete Optimization for Quantum Physics

Max Cut Hamiltonian:
$$\sum(I - Z_i Z_j)$$

Quantum Heisenberg generalization:
$$\sum(I - X_i X_j - Y_i Y_j - Z_i Z_j)$$

Motivation

The Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. Beyond 1 dimension, the properties of the anti-ferromagnetic Heisenberg model are notoriously difficult to analyze.



Anti-ferromagnetic Heisenberg model: roughly neighboring quantum particles aim to align in opposite directions. This kind of Hamiltonian appears, for example, as an effective Hamiltonian for so-called Mott insulators.
[Image: Sachdev, http://arxiv.org/abs/1203.4565]

A new classical algorithm produces approximate solutions for the above quantum model that are mathematically guaranteed to be relatively close in quality to optimal quantum solutions.

First nontrivial rigorous approximations for these problems:
0.498-approx via a product state, where 1/2 is best possible for product states
(also 0.649-approx for XY model, where 2/3 is best possible for product states)

[Gharibian & Parekh; 2018]

Take Away

- Should not expect quantum computers to solve NP-hard problems in polynomial time

- Most quantum optimization approaches are heuristics, though rigorous comparisons with classical are possible in certain settings

- Significant quantum resource advantages over classical for optimization have not been demonstrated in a satisfying way

- Davide will give more examples, including constrained optimization problems, and discuss implementing QAOA-based algorithms as quantum circuits

U.S. DEPARTMENT OF ENERGY | Office of Science

This work was sponsored by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Quantum Algorithm Teams program.