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Quantum Optimization Algorithms

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with

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CIS External Review 2018

Sandia National Laboratories

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Why quantum algorithms?

Sandia National Laboratories

- Potential power of quantum resources is too great to ignore
- **Bold science:** our insights into the unique advantages quantum resources for discrete optimization can shape future quantum systems and applications. Quantum perspective has inspired new classical algorithms!
- **Quantum algorithms to complement, validate, and leverage Sandia's world-class efforts in quantum hardware:** need for quantum applications and algorithms that may be executed on near-term quantum systems. We identify such applications in discrete optimization. Complements quantum testbed efforts.
- Increased external funding agency interest in novel quantum applications and techniques

State of quantum “speedups”

- **Unproven** exponential speedup:
  Shor’s quantum factorization algorithm

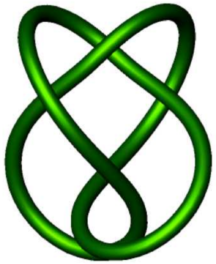
- Provable modest speedup:
  Grover’s quantum search algorithm

- Provable exponential resource advantage in specialized models of computation:
  Query and communication complexity

Limited bag of tricks for speedups

50+ algorithms: http://math.nist.gov/quantum/zoo

Phase Estimation (ca. 1994)



- Factoring
- Quantum chemistry
- Linear systems
- Topological invariants

Amplitude Amplification (ca. 1996)

- Unordered search
- Graph/network properties
- Data collision problems
- Matrix product verification

Hamiltonian Simulation (ca. 1996)

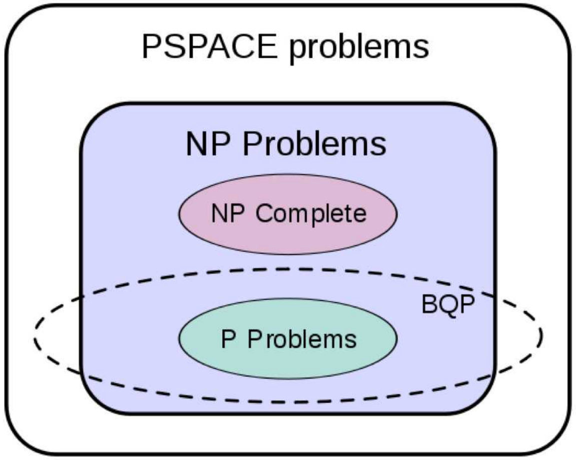
- Quantum chemistry
- Linear systems
- Maze solving

Quantum Walk (ca. 2002)

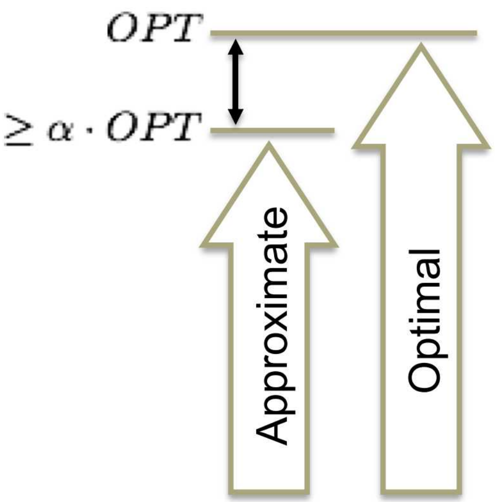
- Boolean formula evaluation
- Spatial search
- Quantum chemistry

New quantum algorithmic approaches are desperately needed!

Quantum Approximation Algorithms: Better instead of just faster



Motivation: hard to efficiently find optimal solutions for NP-complete optimization problems, **even for quantum computers**



Approach: an ***approximation algorithm*** efficiently produces a near-optimal solution with a mathematically provable bound on quality

Innovation: ***quantum approximation algorithms (QAA)*** direct quantum resources towards **higher-quality solutions** instead of faster **running times**, sidestepping barriers to quantum speedups

Approximation Algorithms: Rigorous bounds on performance

A β-approximation algorithm runs in polynomial time, and for any instance *I*, delivers a solution such that:

$$Cost(Solution_I) \geq \beta \cdot Cost(Relaxation_I) \geq \beta \cdot Cost(OPT_I)$$

Heuristics

- Guided by intuitive ideas
- Often perform well on practical instances
- May perform very poorly in worst case
- Often difficult to prove anything about performance

Approximation Algorithms

- Guided by performance proof
- May perform poorly compared to heuristics
- Rigorous bound on worst-case performance
- Designed with performance proof in mind

Quantum bits

State space

Classical bit: (bit)

OR

1 = Head   0 = Tail

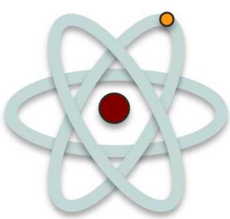
{0, 1}

Prob. bit: (p-bit)

0 with probability $1 - p$
1 with probability p

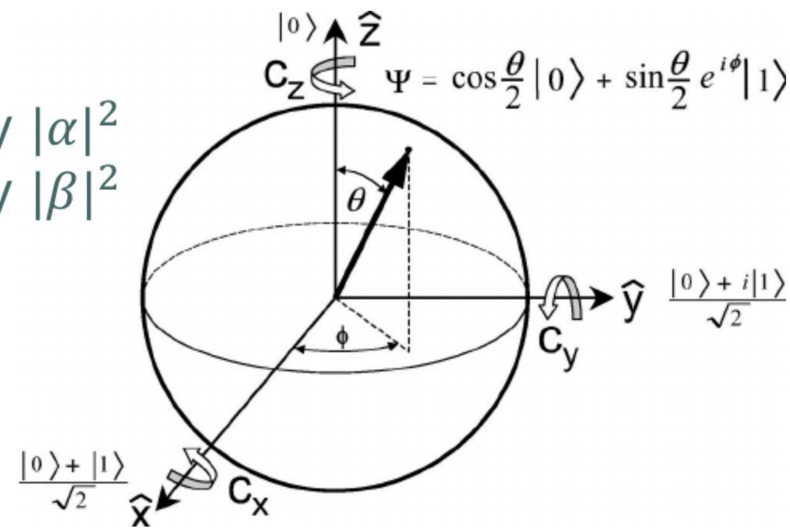
0   p 1

Quantum bit: (qubit)



$$\alpha|0\rangle + \beta|1\rangle$$

0 with probability $|\alpha|^2$
1 with probability $|\beta|^2$



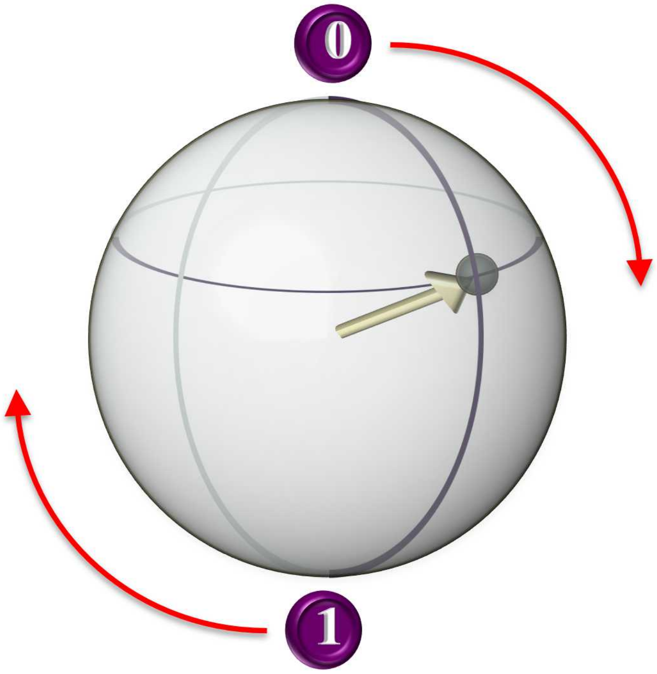
Quantum gates

Can take the "square root" of ordinary logic gates

Conventional logic gate: NOT

$$\text{yes} \rightarrow \text{no}$$

$$\text{no} \rightarrow \text{yes}$$

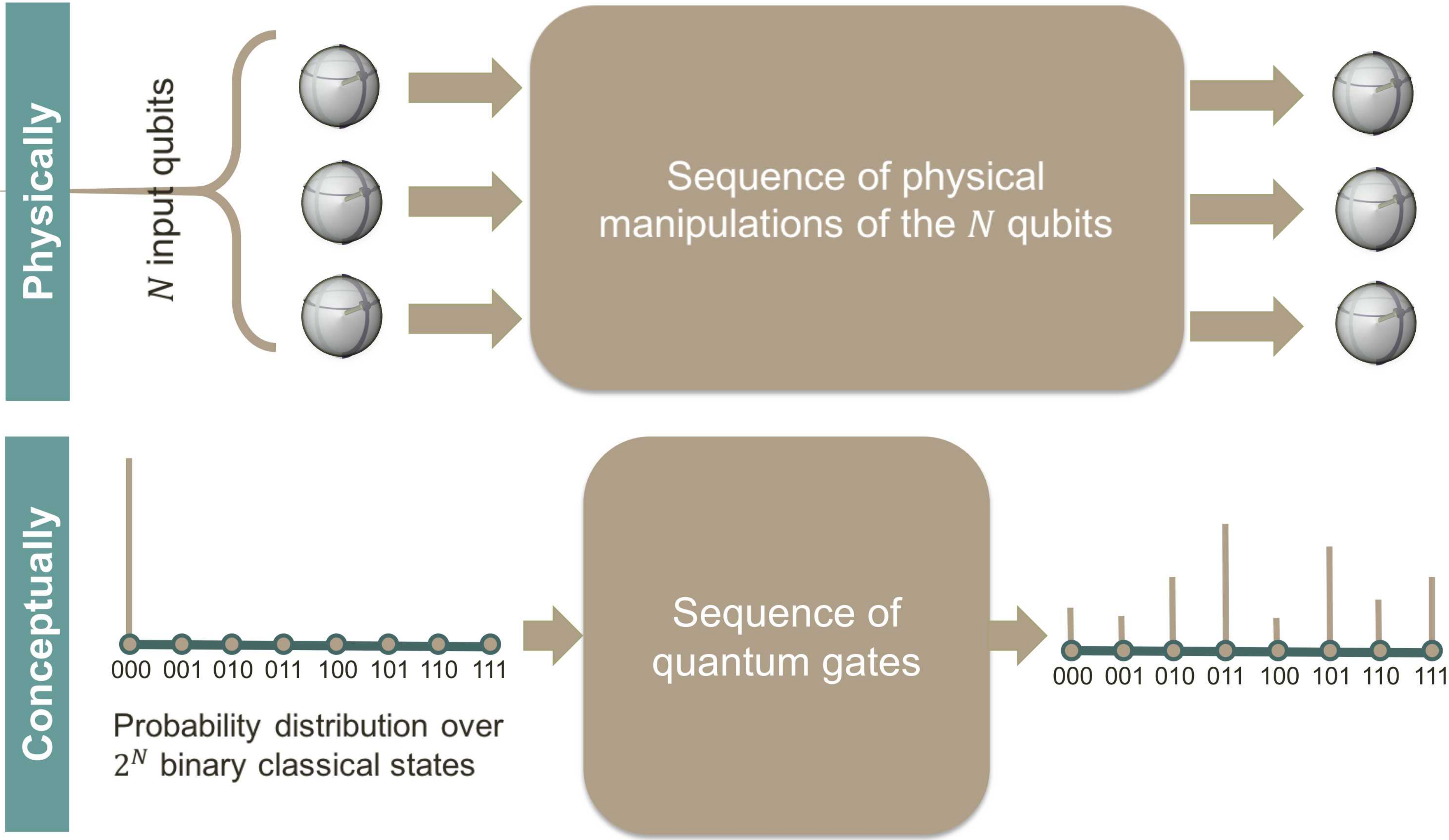


Quantum logic gate: $\sqrt{\mathrm{NOT}}$

$$\text{yes} \rightarrow 50/50 \text{ chance of yes or no}$$

$$\text{no} \rightarrow 50/50 \text{ chance of yes or no}$$

Quantum Algorithms



Quantum Approximate Optimization

The Quantum Approximate Optimization Algorithm (QAOA) was introduced by Farhi et al. in 2014

$$e^{i\sum_i \beta X_i} e^{i\gamma \sum_{ij\in E} Z_i Z_j} |+\rangle^{\otimes n}$$

Only known quantum approximation algorithm framework

Classical approximation algorithms have been studied since the 1960s

- Can be viewed as a discretization of adiabatic quantum computing
- Results in low-depth quantum circuits, suitable for near-term quantum
- Generic framework for discrete optimization problems

[Farhi et al., *A Quantum Approximate Optimization Algorithm*, arXiv:1411.4028, 2014]

Application: Constraint Satisfaction

Maximum SAT is an optimization version of SAT:

$$(x_1 \vee x_2) \wedge (\neg x_1 \vee x_2) \wedge (x_1 \vee \neg x_2) \wedge (\neg x_1 \vee \neg x_2)$$

Impossible to satisfy all 4 constraints, but can satisfy 3 of them.

Max constraint satisfaction seeks to satisfy as many constraints as possible. Constraints may be arbitrary Boolean functions.

Impact on complexity: e.g., 2-SAT is in P, but Max 2-SAT is NP-hard.

Applications: hardware/software verification and validation, VLSI design bioinformatics, data analysis, machine learning

[J. Berg et al., *Applications of MaxSAT in data analysis*, 2015]
[PFM da Silva, *Max-SAT Algorithms For Real World Instances*, 2010]

QAOA for Max 3-XORSAT

Goal of Max 3-XORSAT is to satisfy max number out of *m* given XOR clauses:

$$(x_1 \oplus x_3 \oplus \neg x_4), (\neg x_1 \oplus x_2 \oplus x_3), \ldots$$

Restricted version: each variable appears in at most *d* clauses

Farhi et al. showed that QAOA beats the best known classical approx alg:

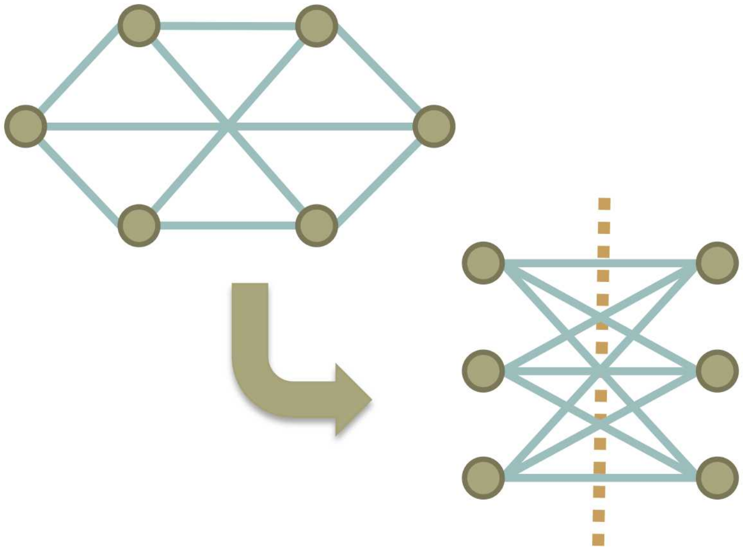
Authors	Year	Result	Type
Trevisan	2000	$\left(\frac{1}{2} + \frac{O(1)}{d}\right) m$	Classical
Farhi et al.	2014	$\left(\frac{1}{2} + \frac{O(1)}{d^{3/4}}\right) m$	Quantum
Barak et al.	2015	$\left(\frac{1}{2} + \frac{O(1)}{\sqrt{d}}\right) m$	Classical
Farhi et al.	2015	$\left(\frac{1}{2} + \frac{O(1)}{\log d \sqrt{d}}\right) m$	Quantum

Barak et al.'s result is best possible up to constants unless P=NP

[Farhi et al., *A Quantum Approximate Optimization Algorithm…*, arXiv:1412.6062v2, 2015]

The Max Cut Problem

Max Cut is a fundamental NP-hard graph partitioning problem

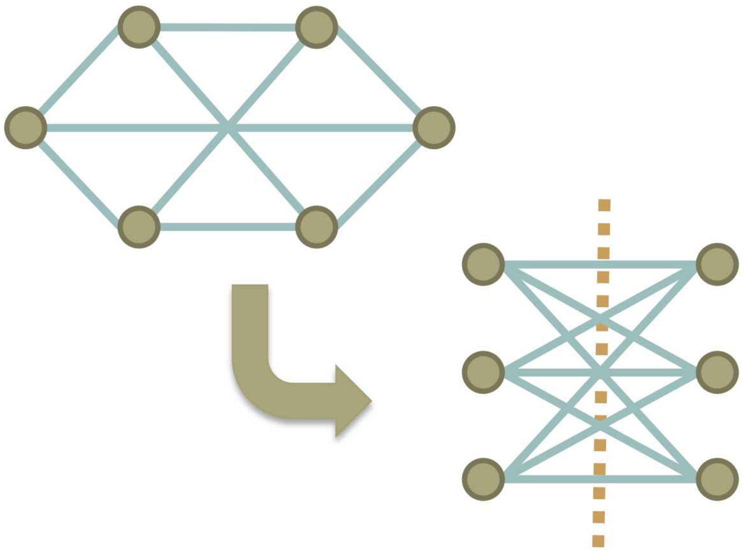


Partition vertices of a(n edge-weighted) graph two parts
to maximize (weight of) crossing edges

QAOA for Maximum Cut

We show that QAOA outperforms best classical algorithm for the well-known Maximum Cut problem on *d*-regular triangle-free graphs with *m* edges

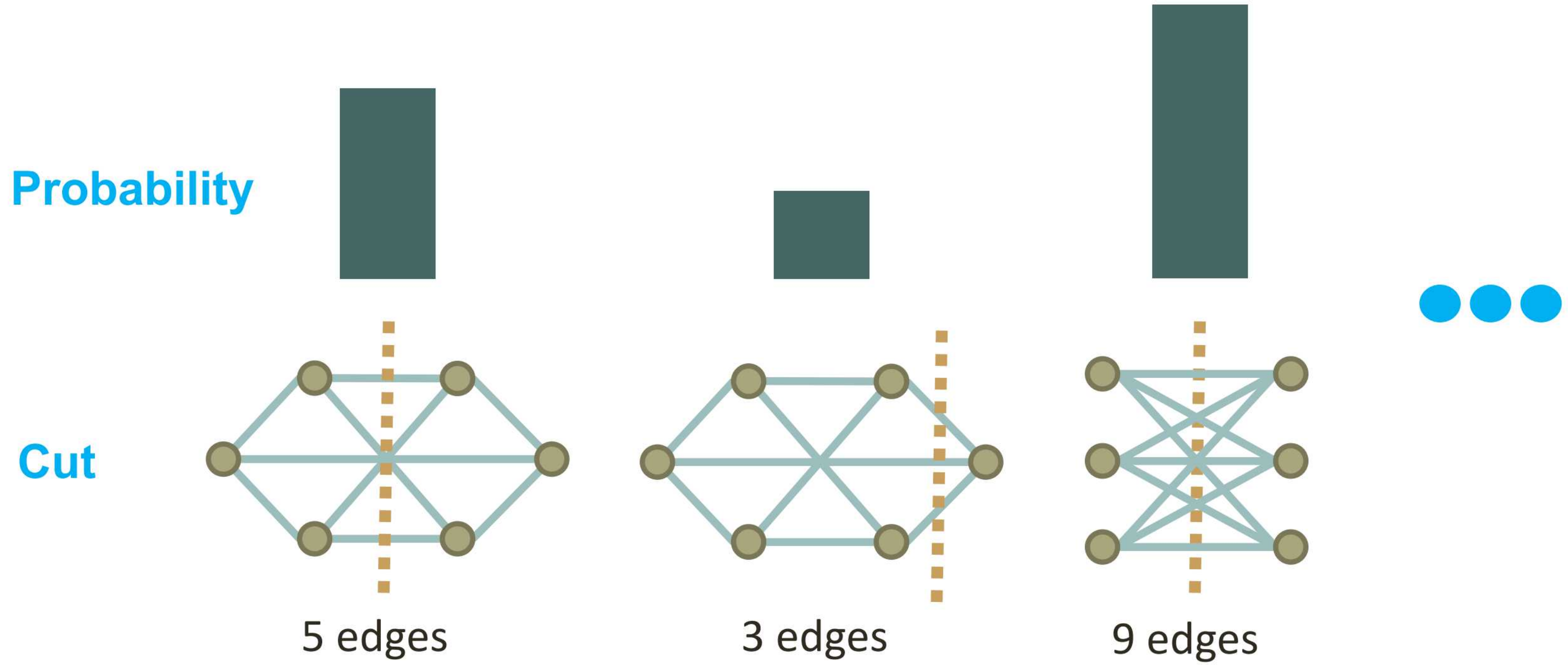
Authors	Year	Result	Type
Shearer	1992	$\left(\frac{1}{2}+\frac{0.177}{\sqrt{d}}\right)m$	Classical
Hirvonen et al.	2014	$\left(\frac{1}{2}+\frac{0.281}{\sqrt{d}}\right)m$	Classical
Parekh et al.	2017	$\left(\frac{1}{2}+\frac{0.303}{\sqrt{d}}\right)m$	Quantum



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

Recovering a cut from our algorithm

Our QAOA-based quantum algorithm samples from a probability distribution on cuts in a graph, likely to yield a cut with many edges



Expectation of QAOA for Max Cut

If $|\boldsymbol{\Psi}(\boldsymbol{\beta}, \boldsymbol{\gamma})\rangle$ be the state produced by QAOA for Max Cut; then:

$$\langle\Psi|Z_i Z_j|\Psi\rangle = \frac{1}{2}\sin^2(2\beta)\cos(\gamma)^{\delta_i+\delta_j-2(n_{ij}+1)}\left(1-\cos(2\gamma)^{n_{ij}}\right) - \frac{1}{2}\sin(4\beta)\sin(\gamma)\left(\cos(\gamma)^{\delta_i-1}+\cos(\gamma)^{\delta_j-1}\right),$$

where δ_i is the degree of vertex i, and n_{ij} is the number of common neighbors of vertices i and j.

Surprising that QAOA expectation may be precisely computed classically!

Quantum Constraint Satisfaction

Classical clause: $(\neg x_i \vee x_j)$

$$\begin{array}{r} \\ x_i, x_j = 0,0 \\ x_i, x_j = 0,1 \\ x_i, x_j = 1,0 \\ x_i, x_j = 1,1 \end{array} \begin{array}{c} \begin{array}{cccc} 0,0 & 0,1 & 1,0 & 1,1 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

2-local Hamiltonian $H_{i,j}$ on i, j

Quantum clause: rank 3

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

$$H_{ij} = I - \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|)$$

Objective is to find max eigenstate of sum of "local Hamiltonians"

$$Max_{\Psi} \left\langle \Psi \middle| \sum H_{ij} \middle| \Psi \right\rangle$$

Hamiltonian eigenstate problems naturally link quantum mechanics and optimization

New *classical* approximation algorithm for quantum Max SAT

$$Max_{\Psi} \langle\Psi|\sum H_S|\Psi\rangle ,$$

where each H_S is a rank $(2^{|S|}-1)$ projector on the qubits in set S

Result: 3/4-approximation, where only a trivial 1/2-approximation was known, based on classical Max SAT approximation (Goemans-Williamson 1994)

Research challenge: find applications for quantum Max SAT, since it is a natural generalization Max SAT (candidates: machine learning, data analysis)

Quantum Max SAT Relaxation

($H_C = I - |\pi_C\rangle\langle\pi_C|$ is the constraint for each set of qubits C)

$$\max \sum_{C \in \mathcal{C}} w_C z_C$$

$$\sum_{i \in S_C} (1 - \langle \pi_C | \rho_i | \pi_C \rangle) \geq z_C, \text{ for all } C \in \mathcal{C}$$

$$z_C \leq 1, \text{ for all } C \in \mathcal{C}$$

$$\text{Tr}(\rho_i) = 1, \text{ for all } i \in V$$

$$\rho_i \succeq 0, \text{ for all } i \in V,$$

quantum: π_c is "bad" space for constraint on C

The above is a semidefinite program, but not obvious this is a relaxation
(i.e., are single-qubit reduced density matrices of a state ρ feasible for the above?)

$$\max \sum_{C \in \mathcal{C}} w_C z_C$$

$$\sum_{i \in S_C^+} x_i + \sum_{j \in S_C^-} (1 - x_j) \geq z_C, \text{ for all } C \in \mathcal{C}$$

$$z_C \leq 1, \text{ for all } C \in \mathcal{C}$$

$$0 \leq x_i \leq 1, \text{ for all } i \in V$$

classical Max SAT relaxation

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Quantum Generalizations of Max Cut

Max Cut constraints:

$$H_{ij} = I - Z_i Z_j$$

Generalization:

$$H_{ij} = I - X_i X_j - Y_i Y_j - Z_i Z_j$$

(maximization version of quantum Heisenberg model)

Most general form we consider:

$$H_{ij} = I - \sum_{\{k=1\}}^{3} (\alpha_{k,i} X_i + \beta_{k,i} Y_i + \gamma_{k,i} Z_i)(\alpha_{k,j} X_j + \beta_{k,j} Y_j + \gamma_{k,j} Z_j)$$

(gives us basically any symmetric H_{ij})

First nontrivial results:

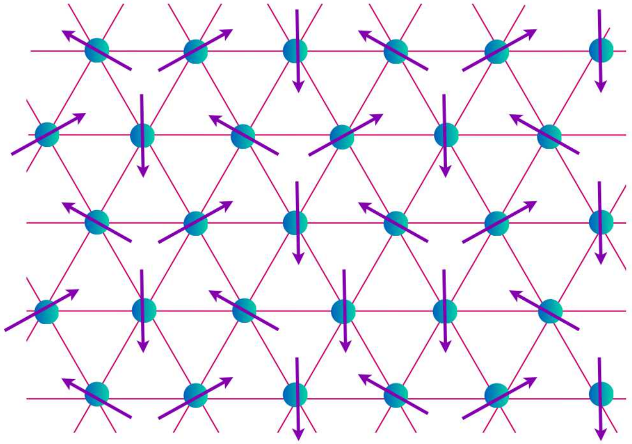
0.498-approx via a product state, where 1/2 is best possible for product states

0.649-approx for XY model, where 2/3 is best possible for product states

Approximate Solutions for Quantum Heisenberg Models via Discrete Optimization

Scientific Achievement

Discrete optimization techniques enable new rigorous approximations of low-energy states of quantum Heisenberg Hamiltonians, a central topic in condensed matter physics.



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)

Significance and Impact

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. Exploiting analytical tools from discrete optimization, a team led by Sandia National Labs has developed new algorithms to rigorously approximate hard-to-compute properties of this model beyond 1-D.

Research Details

– The researchers introduce a new quantum Hamiltonian model that simultaneously generalizes the quantum Heisenberg anti-ferromagnet and hard classical graph partitioning problems.

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

S. Gharibian, O. Parekh, C. Ryan-Anderson, 2018.
Work was performed at Sandia National Laboratories And Virginia Commonwealth University.

Future work: QOALAS

Quantum Optimization and Learning and Simulation

- New DOE/ASCR project funded through ASCR's first quantum algorithms program [FY18-20, $4.5m]
- Developing quantum algorithms for optimization, machine learning, and quantum simulation by unearthing new connections among these areas
- Stellar team consisting of top quantum information scientists and computer scientists from Caltech, LANL, and University of Maryland

Summary

- First or best approximation algorithms for quantum problems arising in condensed matter physics and generalizing classical Boolean satisfiability
- The only known quantum approximation algorithm outperforming the best-known classical algorithm (fundamental graph partitioning problem)
- Success by bridging discrete optimization and quantum information science
- Insights have lead to new funding to develop quantum optimization, quantum machine learning, and quantum simulation algorithms

Outputs

- **Related Publications:**
  - Benchmarking adiabatic quantum optimization for complex network analysis.
    O. Parekh, J. Wendt, L. Shulenburger, A. Landahl, J. Moussa, and J. Aidun
    Technical Report SAND2015- 3025, arXiv:1604.00319, 117 pages, 2015
  - Approximate Constraint Satisfaction in the Quantum Setting.
    Sevag Gharibian, Ojas Parekh, and Ciaran Ryan-Anderson
    26 pages, under preparation for submission to SODA, 2018
- **Selected Presentations:**
  - Investigating the Quantum Approx. Opt. Algorithm's Advantage over Classical Algorithms
    Ojas Parekh and Ciaran Ryan-Anderson
    Selected as a full presentation at the 19th Annual SQuInT Workshop, 2017
  - Quantum Approximation Algorithms
    Ojas Parekh and Ciaran Ryan-Anderson.
    Invited presentation at the SIAM Annual Meeting, 2017
- **Related Funding:**
  - Benchmarking Adiabatic Quantum Computing [FY13-17, SPP, $1m]
  - Quantum Approximation Algorithms [FY16-18, LDRD, $1m]
  - Quantum Optimization and Learning and Simulation (QOALAS) [FY18-20, DOE/ASCR, $4.5m]
  - Benchmarking Quantum Sensor Placement Approaches [FY18-19, SPP, $1m]