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# Quantum gate-model approaches to exact and approximate optimization

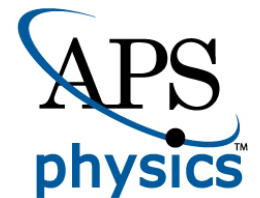
**Stuart Hadfield**



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APS March Meeting, F42: NISQ Applications III. Boston MA, March 5 2019



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# NASA Quantum A.I. Lab (QuAIL)



NASA Ames Research Center  
Moffett Field, Silicon Valley, CA

[ti.arc.nasa.gov/tech/dash/groups/physics/quail/](https://ti.arc.nasa.gov/tech/dash/groups/physics/quail/)

**We are hiring!**

APS March Meeting, Boston MA, March 5 2019



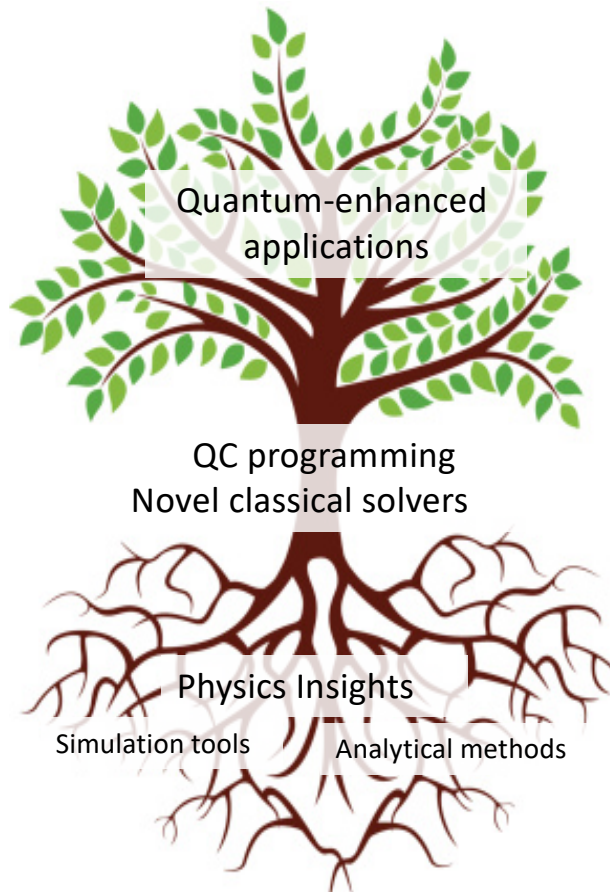
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# Quantum Computing at NASA



- Application focus areas
  - Planning and scheduling,
  - Fault diagnosis
  - Robust network design
  - Machine learning
  - Simulating quantum algorithms and circuits
- Programming quantum computers
  - Quantum algorithm design and analysis
  - Mapping, parameter setting, error suppress
  - Hybrid quantum-classical approaches
- QC ↔ state-of-the-art classical solvers
- Physics-based insights into QC and Machine Learning

**Perspective article:** Biswas, et al.  
A NASA perspective on quantum computing: Opportunities and challenges. *Parallel Computing* 64 (3), 81-98 (2017)





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# The dawn of the quantum (NISQ) era...

Only small number of quantum algorithms known with *established quantum advantage*  
... *Not surprising at this early stage of quantum information processing hardware!*

*How broad will the applications of quantum computing ultimately be?*

**Special case:** What will the be **impact of quantum computers** for **optimization?**

- Optimization problems are ubiquitous in science, engineering, business, etc.
- Tremendous interest in **quantum-enhanced** exact/approximate solvers and heuristics

**In this talk** I'll overview some NASA QuAIL results on **quantum gate-model optimization**, with a focus on applications suitable for **NISQ devices**





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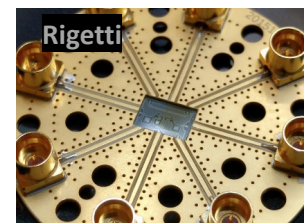
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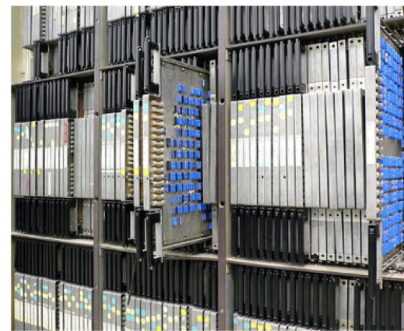
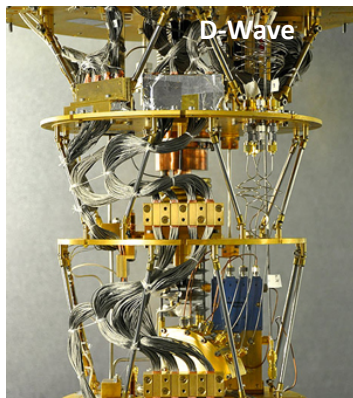
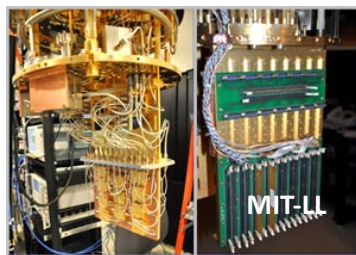


# Emerging quantum devices ...history repeats?

## Gate-model



## Quantum annealers



Illiad IV  
NASA Ames Research Center



Hans Mark, NASA Ames director.  
Brought Illiac IV to NASA in 1972

Illiad IV - first massively parallel computer

- ▶ 64 64-bit FPUs and a single CPU
- ▶ 50 MFLOP peak, fastest computer at the time

Finding good problems and algorithms was challenging.

Would computers ever be able to compete with wind tunnels?



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# Classical heuristics for optimization

Most algorithms run on supercomputers have **not** been mathematically proven to outperform prior algorithms

**Heuristics:** solvation methods where we don't have performance bounds (but may work well in practice)

- Provable bounds hard to obtain!
- Development of classical heuristics typically involves empirical testing: **run and see what happens**  
e.g., competitions for SAT, planning, ML, etc.

Existing quantum hardware has supported only ***extremely limited testing*** of quantum algorithms so far



Pleiades supercomputer  
NASA Ames Research Center

**Conjecture:** *Quantum heuristics for optimization will significantly broaden the applications of quantum computing – in particular NISQ devices*



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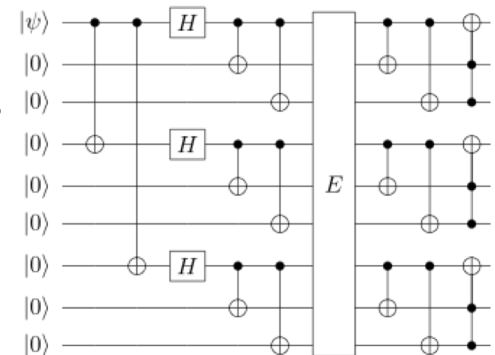
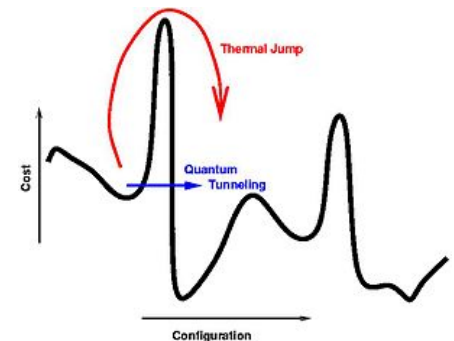
# Quantum approaches to optimization

While **quantum annealing** hardware shows potential, it remains open how much computational speedup it can provide

- Unclear what will be the “**killer applications**” of these devices
- Hardware *locality*, *precision*, and other restrictions cause difficulties
- Currently built/targeted devices are special-purpose, not computationally universal
- No theory of robust fault-tolerance

In contrast, **quantum-gate model** devices appear to offer **advantages**

- **Sophisticated techniques/subroutines:** Can implement much more diverse operators
  - e.g., Hamiltonian **simulation**, operator **compilation**, ancilla-assisted-ops, RUS
- Locality / qubit connectivity may be **much less of a bottleneck**
- Robust theories of **error correction / fault-tolerance**
- **Gate-model heuristics much less studied** up to now! Especially **empirically**







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# Quantum approaches to optimization

Some applicable quantum approaches:

(Not exhaustive!!)

- Quantum annealing / Adiabatic optimization [e.g. Nishimori et al., Farhi et al.]
- Grover's / speedup of expo time algorithms [e.g. Montanaro, Ambainis et al.]
- Quantum SDP solvers [e.g. Brandão et al.]
- ⋮
- Variational Quantum Eigensolver (VQE) [Peruzzo et al.]
- **Quantum Approximate Optimization Algorithm (QAOA)** [Farhi, Goldstone, Gutmann 2014]

Low-depth QAOA appears especially suitable for running on **NISQ gate-model devices**



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# QAOA @ APS2019: $\geq 11$ talks!

11 Results Found.

C42.00009 [Quantum Local Search for Graph Community Detection](#)

C42.00012 [Experimental Methods for Improving Heuristic Quantum Algorithms on NISQ Devices](#)

F27.00004 [Quantum Circuit Compilation to NISQ processors](#)

F42.00003 [Variational Approaches for Quantum Simulation](#)

F42.00004 [Quantum gate-model approaches to exact and approximate optimization](#)

G70.00371 [Optimal Quantum Approximate Optimization Algorithm: Success Probability and Runtime Dependence Depth](#)

K27.00002 [Performance of the Quantum Approximate Optimization Algorithm on the Maximum Cut Problem](#)

K42.00002 [How many qubits are needed for quantum computational supremacy?](#)

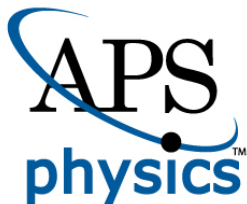
K42.00004 [Variational Quantum Factoring](#)

V36.00003 [Engineering Trapped-Ion Systems for Large Scale Quantum Simulation](#)

X28.00012 [Low-depth parallelization of k-local gates and applications](#)

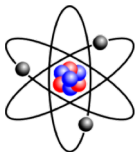
Search:

Word search of titles and abstracts only.





# Parameterized Quantum Circuits for Optimization



## Quantum computer:

1. Input  $\ell$  parameters  $\gamma_1, \dots, \gamma_\ell \in [0, \pi]$
2. Prepare initial state  $|s\rangle$  e.g.,  $|s\rangle = |+\rangle^{\otimes n}$
3. Create a **parameterized quantum state**  
 $|\gamma_1, \gamma_2, \dots, \gamma_P\rangle = Q(\gamma_1, \dots, \gamma_P)|s\rangle$
4. Measure in the computational basis to obtain a candidate solution  $x^*$  with cost function value  $C(x^*)$

Parameters  $\gamma_1, \dots, \gamma_P$

Measurement outcomes  
(candidate solutions)

**Problem:** Given a cost function  
 $C: \{0, 1\} \rightarrow \mathbb{R}$   
find a string  $x$  maximizing  $C(x)$

**Output: Best solution found**

## Classical computer (controller):

1. Select  $2p$  angles  $\gamma_1^{(j)}, \gamma_2^{(j)}, \dots, \gamma_p^{(j)}$  for each run  $j$
2. Run quantum circuit many times to obtain statistics
3. Use measurement information to **update parameters**
4. Repeat



**NISQ era:** trade-offs between “quality” of quantum device, and required classical processing...

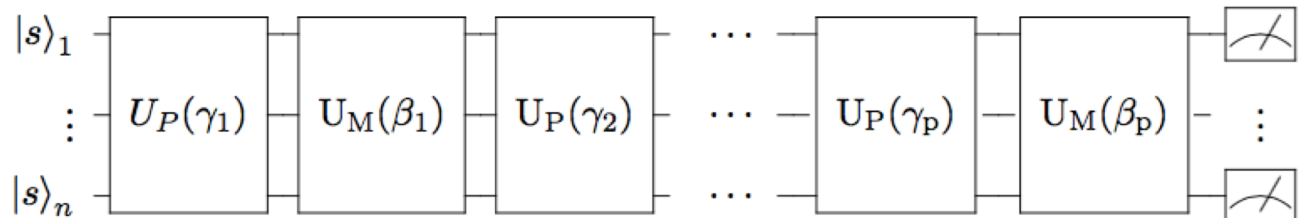




$$(X_j := \sigma_X^j)$$

# Quantum Approximate Optimization Algorithm

QAOA(p) circuit:



Creates quantum state  $|\gamma\beta\rangle$  parameterized by  $2p$  angles  $\gamma_1, \beta_1, \dots, \gamma_p, \beta_p \in [0, \pi]$

**3 main ingredients:**

Phase op.: Evolve under cost Hamiltonian  $C|x\rangle = c(x)|x\rangle$ ,  $U_P(\gamma) = \exp(-i \gamma C)$

Mixing op.: Evolve under transverse-field  $B = \sum_j X_j$ ,  $U_M(\beta) = \exp(-i \beta B)$

Initial state: equal superposition state  $|s\rangle = |+\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{y \in \{0,1\}^n} |y\rangle$



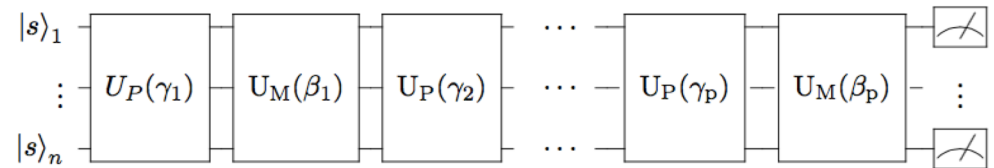
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# QAOA



**QAOA(p) circuit:** Creates quantum state  $|\gamma\beta\rangle$  with  $\gamma_1, \beta_1, \dots, \gamma_p, \beta_p \in [0, \pi]$

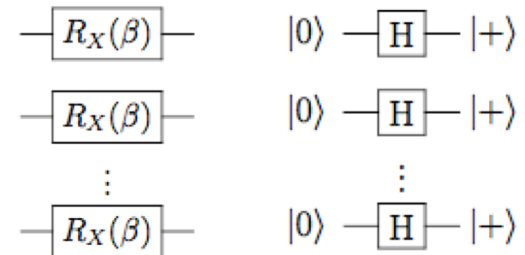
$$|\gamma_1\gamma_2 \dots \gamma_p\beta_1\beta_2 \dots \beta_p\rangle = U_M(\beta_p) U_P(\gamma_p) U_M(\beta_{p-1}) \dots U_M(\beta_1) U_P(\gamma_1) |s\rangle$$

*Achievable circuit depth p improves with better hardware!*

**Phase op.:** Can often be implemented inexpensively...

e.g. MaxCut:  $C \simeq \sum_{(jk)} Z_j Z_k$

**Mixing op.:** Can be implemented in depth 1 with X-rotation gates



**Initial state:** Preparable with Hadamards in depth 1



# Constructing phase operators

Given  $f: \{0, 1\}^n \rightarrow \{0, 1\}$  (or  $\rightarrow \mathbb{R}$ ), how to map to  $n$ -qubit Hamiltonian  $H_f$  ?

Boolean or real functions **uniquely** expressed as linear monomials of  $Z_j$  (spin) ops

## Base case: Boolean clauses

$f(x)$	$H_f$
$x$	$\frac{1}{2}I - \frac{1}{2}Z$
$x_1 \oplus x_2$	$\frac{1}{2}I - \frac{1}{2}Z_1Z_2$
$x_1 \wedge x_2$	$\frac{1}{4}I - \frac{1}{4}(Z_1 + Z_2 - Z_1Z_2)$
$x_1 \vee x_2$	$\frac{3}{4}I - \frac{1}{4}(Z_1 + Z_2 + Z_1Z_2)$
$\overline{x_1x_2}$	$\frac{3}{4}I + \frac{1}{4}(Z_1 + Z_2 - Z_1Z_2)$

## Composition rules

$$H_{\neg f} = H_{\bar{f}} = I - H_f$$

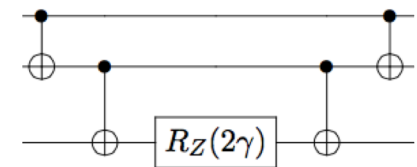
$$H_{f \wedge g} = H_{fg} = H_f H_g$$

$$H_{f \oplus g} = H_f + H_g - 2H_f H_g$$

$$H_{f \vee g} = H_f + H_g - H_f H_g$$

$$H_{af+bg} = aH_f + bH_g \quad a, b \in \mathbb{R}$$

## Circuit Compilation



$$U = e^{i\gamma Z_1 Z_2 Z_3}$$

Many useful results for diagonal Hamiltonians, **and (mixing) unitaries**, follow from the Fourier analysis of Boolean functions





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# Power of QAOA Circuits?

- Provable **Grover's speedup**: QAOA circuits can search  $N$  items using  $O(\sqrt{N})$  queries  
Z Jiang, EG Rieffel, Z Wang. PRA (2017)
- Lloyd recently showed QAOA **quantum computationally universal**  
S Lloyd. *arXiv:1812.11075* (2018)

On the other hand, **how powerful are low-depth QAOA circuits?**

- Shown to be **computationally hard** to efficiently classically sample from the output of QAOA circuits **even for lowest depth  $p=1$**  case  
E Farhi, AW Harrow.. *arXiv:1602.07674* (2016)
- QAOA( $p=1$ ) **gave best approximation algorithm known (!)** for E3LIN2  
Farhi et al, *arXiv:1414.6062* (2014)  
.... **Only to inspire an even better classical algorithm**  
Barak et al. *arXiv:1505.03424* (2014)

**To what extent is QAOA a promising optimization approach? Important open problem!**

- Many **new applications** discovered – sampling, state prep, ML, etc. – see APS talks!

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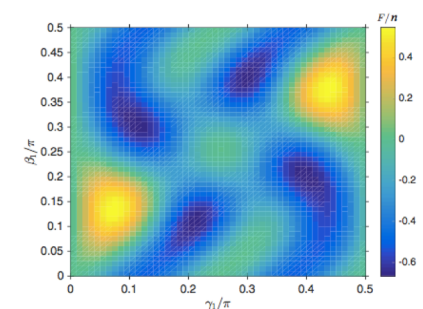
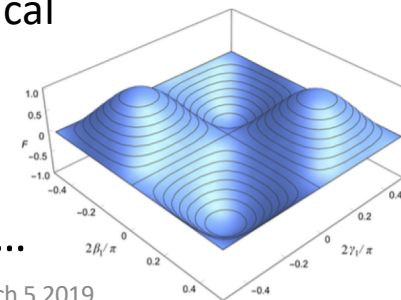
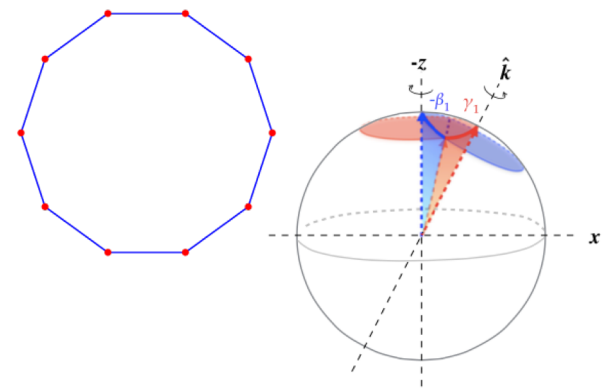
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# QAOA: *quantitative* insights from physics

Z Wang, SH, Z Jiang, EG Rieffel. PRA (2018)

- For **MaxCut** on a **ring graph**, QAOA dynamics can be mapped to **non-interacting Fermions**
  - This analysis gives insight into the *energy landscape*, *symmetries*, and *parameter setting*
- For **MaxCut** on **general graphs**, we can derive **analytic performance bounds** using the Heisenberg representation
  - E.g.  $p = 1$  QAOA on  $k$ -regular graphs
  - For **small  $p$** , reproduces **analytically** the numerical results from original QAOA paper
- Our technique extends to  $p > 1$ , but appears difficult to obtain general performance bounds...



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# QAOA: small angle approximations

SH, T Hogg, et al. (2019)

For general  $C: \{0, 1\}^n \rightarrow \mathbb{R}$ , can define “differentials”:

$$\partial_j C(x) = C(x^{(j)}) - C(x) \quad j = 1, \dots, n$$

$x^{(j)}$  means  $x$  with  
its  $j$ th bit flipped

$$D_C(x) = \sum_{j=1}^n \partial_j C(x)$$

These are **diagonal** – so as we saw we can lift to diagonal Hamiltonians  $\partial_j, D_C$

**Theorem.** For  $p = 1$  QAOA with  $|\gamma|, |\beta| \ll 1$ , to **second-order** we have

e.g., valid in  
“Trotterized”  
regime!

$$\langle C \rangle_1 - \langle C \rangle_0 = -\frac{2}{2^n} \gamma \beta \sum_x C(x) D_C(x) + O(\{\gamma, \beta\}^3)$$

*Thus, for small angles, up to sign, initially probability flows from lower cost to higher cost states proportional to the “total differential”  $D_C(x)$  at each  $x$*



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S. Hadfield, Z. Wang, B. O'Gorman, E. G. Rieffel, D. Venturelli, R. Biswas. *Algorithms*, 12(2), 34 (2019)

# From QAOA to the Quantum Alternating Operator Ansatz

**Constrained optimization:** many problems have **hard constraints** - **must** be satisfied

- May come from **problem definition**, or from **problem encoding** or **hardware embedding**
  - e.g. Find  $\max_y c(\mathbf{y})$  such that  $\mathbf{g}(\mathbf{y}) = \mathbf{0}$  ( $\mathbf{g} = \mathbf{0}$  encodes feasible solutions)
    - e.g. Maximum Independent Set, Scheduling Problems, Partitioning...

No adiabatic  
condition  
generally in  
QAOA!

Penalty term approaches (common in QA/AQO) **face difficulties for QAOA!**

- How to deal with “leakage” of probability amplitude into infeasible subspace?

An alternative and possibly more effective approach is to directly **design mixing operators that constrain quantum evolution to stay within the feasible subspace**

- Related to, but much more general than, proposed **alternative driver approach for annealing**

Hen et al., arXiv:1508.04212, arXiv:1602.07942

**Design criteria:** QAOA mixers must i) **preserve feasibility** ii) **connect all feasible states**

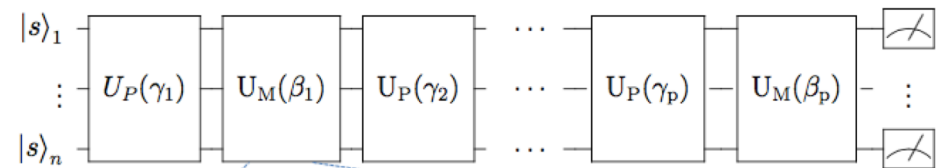
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# Quantum Alternating Operator Ansatz (QAOA)

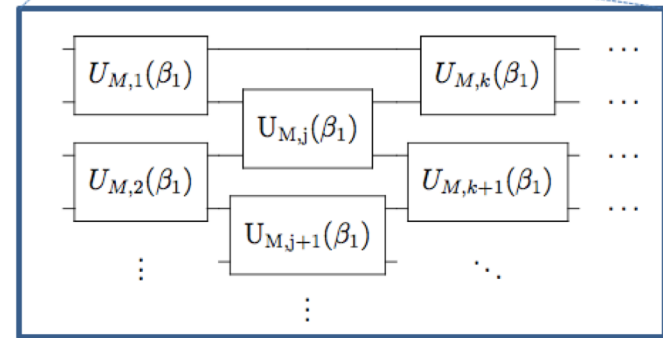
We generalize the QAOA protocol to include much more general families of **parameterized unitary operators**



QAOAnsatz circuit:

Phase op.: Evolve under cost Hamiltonian **or proxy**

Mixing op.: **composite circuit of local unitaries**



$$U_M(\beta) = U_1(\beta)U_2(\beta) \dots U_\ell(\beta)$$

Importantly, in general  $[U_j, U_k] \neq 0$

Initial state: generalize to allow **any easily preparable feasible state**

- May also **generate** from an initial application of the mixing operator to a basis state



# Quantum Alternating Operator Ansatz (QAOA)

Mixing op.: *composite circuit of local unitaries*

$$U_M(\beta) = U_1(\beta)U_2(\beta) \dots U_\ell(\beta)$$

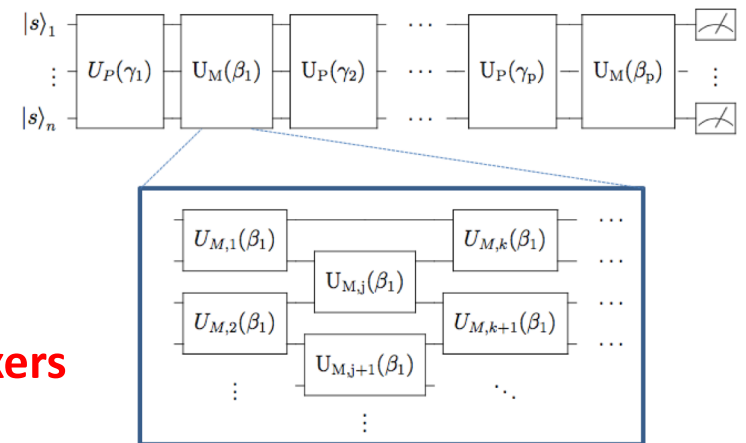
We call each  $U_j(\beta)$  a *partial mixer*

Mixers constructed as **ordered products of partial mixers**

Importantly, in general,  $[U_j, U_k] \neq 0$

- Such a mixer does not correspond to the exponential of a single Hamiltonian, as a family
- Different possible orderings of partial mixers result in **different inequivalent mixers**
  - For NISQ devices, can, e.g., choose ordering with lowest circuit depth

***Our ansatz generalizes QAOA to a much richer class of parameterized quantum states!***





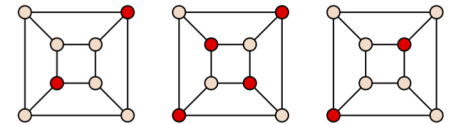
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# Ex: Maximum Independent Set



Given a graph  $G = (V, E)$ , find largest edge-disjoint subset of vertices  $S \subset V$

NP-hard!

Represent with  $\mathbf{n} = |V|$  binary variables mapped to  $\mathbf{n}$  qubits.

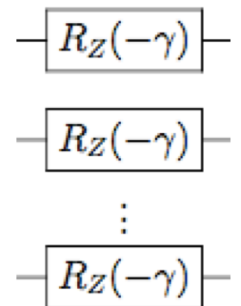
Variable  $x_u = 1$  indicates vertex  $u \in S$

**Initial state:** Empty set  $S = \emptyset$  feasible and trivial to prepare as  $|00 \dots 0\rangle$

Feasibility assumption greatly simplifies phase operator!

**Phase Op.:** cost function to maximize  $c(S) = |S| = \sum_{u \in V} x_u$

maps to Hamiltonian  $C = \frac{n}{2} I - \frac{1}{2} \sum_u Z_u$



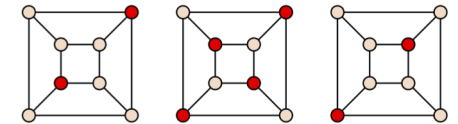
$\Rightarrow U_P(\gamma)$  implementable in **depth 1** with **Z**-rotations:

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$$U_P(\gamma) = \prod_{u \in V} R_{Z_u}(-\gamma)$$



# Ex: Maximum Independent Set



Often ensure feasibility by constructing **partial mixers** from classical **reversible** local moves

Reversible Mixing Rule: Vertex  $u$  can always be added (or removed) if none of its neighbors are in the set

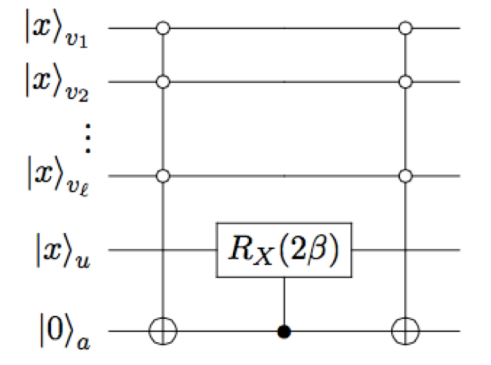
- Can show any two solutions connected by a number of these moves

Reversible Partial Mixing Hamiltonians:  $B_u = (\bar{x}_{v_1} \bar{x}_{v_2} \dots \bar{x}_{v_\ell}) \cdot X_u$  where  $v_j \in \mathbf{nd}(u)$

- Combines **Boolean logic** with **bit-flip** operation
- Partial mixers become **controlled quantum operations**

$$U_u(\beta) = \exp(-i\beta B_u) = \Lambda_{\bar{x}_{v_1} \bar{x}_{v_2} \dots \bar{x}_{v_\ell}}(X_u)$$

- Implementable with  $\mathcal{O}(|\mathbf{ndhd}(u)|)$  basic gates and 1 ancilla
- Many different compilations to quantum gates are possible!



Overall mixing operator:  $U_M(\beta) = \prod_{u \in V} \exp(-i\beta B_u)$  implementable with  $\mathcal{O}(|E|)$  basic gates





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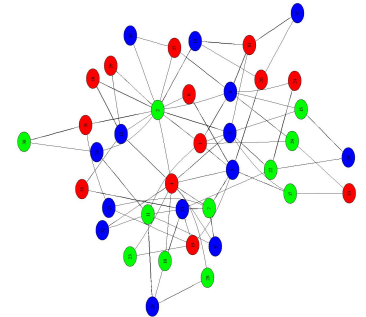
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# Ex: Graph k-coloring problem

Given a graph  $G = (V, E)$ , and  $k$  colors  $1, \dots, k$ , find a vertex color assignment **maximizing the # of properly colored edges**

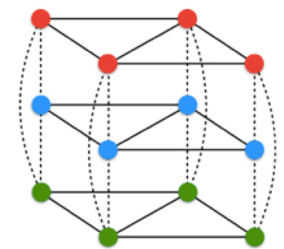
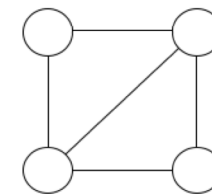
NP-complete decision problem “Is  $G$   $k$ -colorable?”



Unary “one-hot” encoding: use  $k$  qubits for each vertex,  $nk$  qubits total

$$x_{ui} = 1 \text{ iff vertex } u \text{ is colored } j$$

e.g.,  $|100\rangle = \text{blue}$ ,  $|010\rangle = \text{red}$ ,  $|001\rangle = \text{green}$



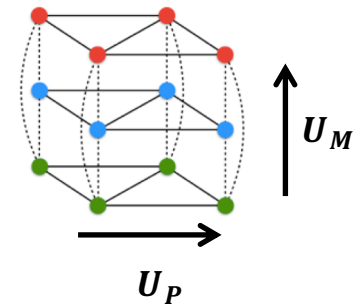
Here **hard constraints come from encoding**

Feasible states are valid colorings (one color per vertex)



# Ex: Graph k-coloring problem

**Initial state:** any valid coloring (e.g., a trial solution),  
or a superposition of all colorings (“W-states”)



**Phase operator:** Objective function

$$C(x) = m - \sum_{(uv) \in E} \sum_{i=1}^k x_{ui} x_{vi}$$

- Straightforward to implement  $U_p(\gamma) = \exp(-i\gamma C)$  with  $Z$ -rotations and CNOTs

**Partial mixing Hamiltonian:**  $B_v = \sum_{i=1}^k X_{v,i} X_{v,i+1} + Y_{v,i} Y_{v,i+1}$

- This Hamiltonian **preserves Hamming weight** (closely related to SWAP)

“XY Model on a Ring”

**Mixing op.:** Therefore, the mixer  $U_B(\beta) = \prod_j \exp(-i\beta B_j)$  **preserves feasibility**

- Can show ‘ring’ structure of  $B_v$  sufficient to reach all colorings
- Could also use ‘fully-connected XY model’, at higher cost (...but better mixing?)



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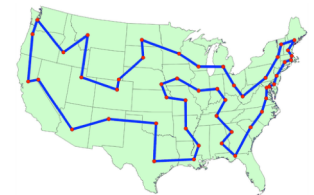


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# Quantum Alternating Operator Ansatz: Applications

- We show constructions for a variety of problems incorporating a diverse set of **encodings** and **hard constraints**, and propose **different mixer designs**
- Our approach leads to **partial mixers utilizing control**, and in combination with other operations beyond the simple bit-flip mixer (e.g. controlled-XY)
- **e.g. Traveling salesman**: states encode **permutations** of the vertices
  - Different mixing operators with **different tradeoffs** are possible
- Our constructions require being able to **efficiently find at least one initial feasible state**  
Typically true, but not always the case for some classes of problems!



SFO <--> BOS



# Quantum Alternating Operator Ansatz: Applications

See the paper for details, many more examples, and resource estimates!

## Controlled-bit-flip mixers

- ▶ Max Independent Set
- ▶ Max Clique
- ▶ Max Vertex Cover
- ▶ Max Set Packing
- ▶ Min Set Cover

## Controlled-bit-flip mixers

- ▶ Max Colorable Subgraph
- ▶ Min Graph Bisection
- ▶ Max Graph Bisection
- ▶ Max Set Packing
- ▶ Max Vertex  $\kappa$ -Cover

## Controlled-XY mixers

- ▶ Max- $\kappa$ -colorable Induced Subgraph
- ▶ Min Graph Coloring
- ▶ Min Clique Cover

## Permutation mixers

- ▶ Traveling Salesperson (TSP)
- ▶ Single Machine Scheduling (SMS), minimizing total weighted squared tardiness
- ▶ SMS, minimizing total weighted tardiness
- ▶ SMS, with release dates

QAOA <sub>p</sub> Problem	# of Qubits	# of Basic Gates
Quadratic Unconstrained Binary Optimization	$n$	$O(p(m+n))$
Max Independent Set	$n+1$	$O(p(m+n))$
Max $k$ -Colorability (Max $k$ -Cut)	$kn$	$O(pk(m+n))$
Max $k$ -Colorable Induced Subgraph	$(k+1)n+1$	$O(p(km+n))$
Min Chromatic Number ( $k = D_G + O(1)$ )	$(n+1)k+1$	$O(p(k^2m+kn))$
Traveling Salesman	$n^2$	$O(pn^3)$
Single Machine Scheduling (Min Total Tardiness)	$nP$	$O(pn^2P)$





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# Gate-model optimization: Future research

As in **quantum annealing**, many of the key **problems remain open** for **gate-model** approaches to quantum optimization

- **Parameter setting** / scheduling
- **Initial states** – how to select ‘best’?
- Design of ‘good; **mixing operators and tradeoffs**
- **Compilation...**
- Ideal vs. real-world **hardware** performance
  - **Robustness** to error / noise resilience?

**Quantum advantage:** When do quantum computers give **speedups** for optimization? Or **better quality** approximations in the same time?

- **New approaches / algorithms?**

For **which classes of problems** are **NISQ** devices likely to prove useful?

- **QAOA and beyond!**

- How can we design quantum algorithms to **best take advantage of real-world hardware?**
- For our QAOA mappings, **the most important question – performance – remains open**. We are excited as bigger and better quantum hardware enables **further empirical experimentation!**
- Further applications of QAOA circuits?
- Further generalizations of our approach?



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# Summary

Can quantum computers enhance the success & scope of NASA missions?

- Many potential applications!

Our ***Quantum Alternating Operator Ansatz*** greatly extends the applicability of the QAOA

- We have achieved partial results, however, there is still much work to be done to **better understand the performance of the algorithm**

We expect **empirical testing** on current and upcoming **NISQ devices** will allow for a much better understanding of the physics and performance of QAOA

- It is important to quantify tradeoffs and which “quantum resources” key for optimization

We are further optimistic that empirical testing on increasingly more powerful quantum systems will be vital towards the understanding and design of **new quantum algorithms for optimization**



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## For overviews of NASA QuAIL research:

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# + We are hiring!



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