18-819F: Introduction to Quantum Computing
47-779/47-785: Quantum Integer Programming & Quantum Machine Learning

NISQ Optimization

Lecture 12

2022.10.12

Agenda

- A Quantum Optimization Algorithm
- Quantum Adiabatic Algorithm
- Adiabatic Quantum Computing
- Quantum Approximate Optimization Algorithm (QAOA)
- QAOA for Constrained Optimization Problems
- Quantum Alternating Optimization Ansatz
- QAOA in the Real World
- Amazon Braket Exercise

Important Previous Lectures

Ising Model and QUBO problems

Lecture 08

09.28.2022

Quantum Annealing, Quantum-Inspired Heuristics, , Benchmarking, and Parameter setting

Lecture 9

10.03.2022

Introduction to Quantum Gates and Circuits

Lecture 11

2022.10.10.

Two ways to execute quantum algorithms: ANALOG or DIGITAL

ANALOG: the algorithm consists of a "schedule" for time-dependent signals, corresponding to Schroedinger Evolution

DIGITAL: the algorithm is "clocked": decomposed into individually calibrated gates that are acting on k-qubits at a time

High level operation of a basic QPU

Initialization of a qubit register

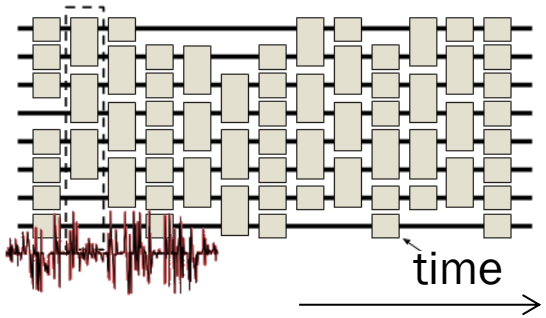
$|0000....\rangle$

The initial reset of the computer is an irreversible operation that dissipates heat

Coherent Quantum Operations

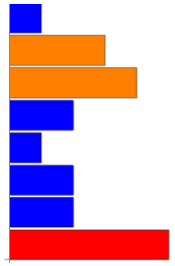
$U_n...U_3U_2U_1|0000....\rangle$

$$|\psi^I(\Delta t)\rangle = T\exp\left(-\frac{i}{\hbar}\int_0^{\Delta t}\hat{H}_c^I(t)\,dt'\right)|\psi^I(0)\rangle$$



Measurement of aregister in the computational basis

$P_{00..00}$ $|0000....00\rangle$
$P_{00..10}$ $|0000....01\rangle$
$P_{00..10}$ $|0000...10\rangle$
$P_{00..11}$ $|0000....11\rangle$
...
$P_{11..11}$ $|1111....11\rangle$



The measurement can be repeated many times to gather a statistics.
The distribution is used either as:

- Algorithm output
- Change parameters for gates for next iteration
- Error correction

The operations are unitary schroedinger evolutions "gates" of single and two qubit gates (but there is noise).
Reversible, zero dissipation.
Operations "use" entanglement, superposition, interference, tunneling etc.

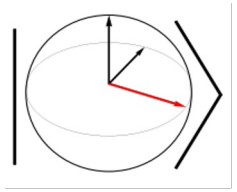
A Quantum Optimization Algorithm Template

1) Map a QUBO Objective function into Ising form and assign the logical identity of each spin variable to a qubit in the processor.

$$\boldsymbol{x_i = (si + 1)/2 \rightarrow |xi\rangle}$$

2) Apply single-qubit rotations to every qubit to put the state of the QPU in superposition of all possible solutions of the optimization problem (Hadarmard gates)

$$|\Psi\rangle_{N\ qubits} = \frac{1}{\sqrt{2^N}} \sum_{n=1}^{2^N} |solution(n)\rangle_n$$



(3) Apply continuous signals, pulses of two level gates and single qubits rotations to change the state, having some smart idea on how to increase the value of $|\Psi_{n=target}|^2$

Algorithms are difficult to design because you are doing matrix multiplication with matrices of dimensions $2^N \times 2^N$– nature does it for you! you don't need to do it but good luck simulating it

(4) Measure the state, read the qubits (they are a single bitstring after measurement) and hope to find the target(s).

(5) Repeat the procedure many times and keep the best result.

The Quantum Adiabatic Algorithm

AQC is based on a property of the time-dependent Schrödinger equation – the «adiabatic theorem».

Einstein's "Adiabaten hypothese": "If a system be affected in a reversible adiabatic way, allowed motions are transformed into allowed motions" (Einstein, 1914).

(1) Switch on a quantum interaction in your system

(2) Take the spectrum of possible energies of your quantum system as a function of the degrees of freedom and set the state to a well-defined energy (not metastable states) which is ranked n^{th} in order of magnitude (e.g., the second smallest)

(3) Do any Schrödinger evolution (no measurement! no noise!) that changes the energy states «sufficiently slow».

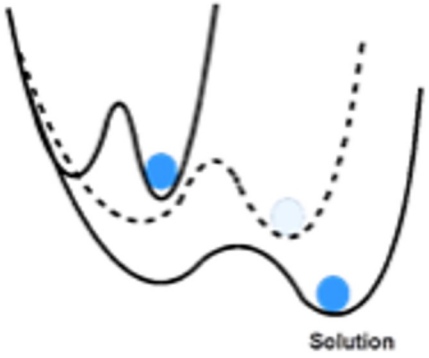
(4) Measure the energy of the state. You will find with 100% probability that the energy is ranked also n^{th}

Adiabatic evolution (e.g., Slow Schrödinger) preserves the energy ranking of your system. The smallest energy state (ground state) also maps into the ground state at the end.

IDEA: map objective function into energy. Start from easy problem to solve with known solution and modify slowly to difficult. Measure unknown solution

Albash, Lidar
Rev. Mod. Phys. 90, 015002 (2018)
https://arxiv.org/abs/1611.04471

- Apolloni 1989
- Finnila 1994
- Nishimori 1998
- Brooke 1999
- Fahri 2001



Adiabatic evolution

Solving ISING/QUBOs using Quantum Computing – How?

Adiabatic Quantum Computing

1. Write objective function into energy of a Quantum System (ISING=QUBO⊂MINLP).
2. Start from easy problem to solve with known solution and modify slowly to difficult.
3. Measure unknown solution

- Property of time-dependent Schroedinger equation – the «adiabatic theorem».

Using different models of Quantum Computers

- Gate-based computers
  - For solving QUBOs, we can use algorithms like:
    - Quantum Approximate Optimization Ansatz (QAOA)
    - Variational Quantum Eigensolver (VQE)
  - For optimization, algorithms can be understood as discretized adiabatic computation
  - IBM/Google/Rigetti/IonQ/Quantinuum quantum computers are gate-based
- Quantum annealers
  - They run a single quantum algorithm, quantum annealing
  - Finite temperature implementation of adiabatic quantum evolution
  - Analog computation
  - D-Wave quantum annealer is the best-known example

Quantum Approximate Optimization Algorithm

QAOA Tutorial Outline

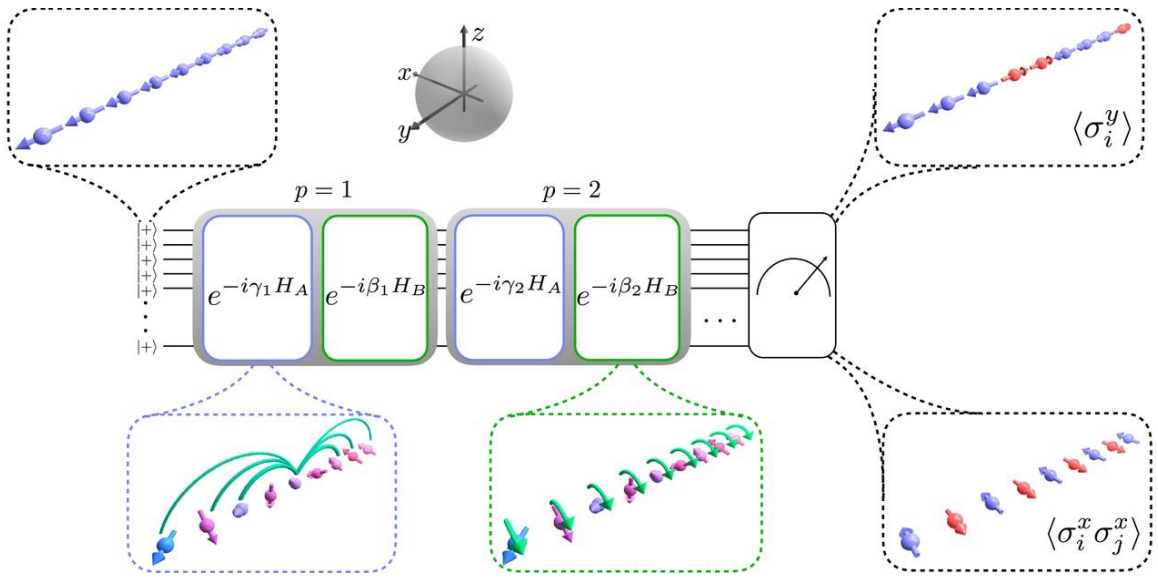
- Quantum Approximate Optimization Algorithm: review and status
- The «Quantum Alternating Operator Ansatz»
  - Mixing Operators
  - Examples
- Compiling and Executing
  - The gate synthesis problem
  - Review of compilation methods
  - Compiling framework in nearest-neighbor architectures

READING LIST

- **Quantum Approximate Optimization with Hard and Soft Constraints.** Hadfield, S., Wang, Z., Rieffel, E. G., O'Gorman, B., Venturelli, D., & Biswas, R. (2017, November). In *Proceedings of the Second International Workshop on Post Moores Era Supercomputing* (pp. 15-21). ACM.
- **From the quantum approximate optimization algorithm to a quantum alternating operator Ansatz** Hadfield, S, Z. Wang, B. O'Gorman, E. G. Rieffel, D. Venturelli, and R. Biswas. *arXiv preprint arXiv:1709.03489 (2017)*. Algorithms (2019).
  - **Best Paper Award MDPI Algorithms Journal**

Quantum Approximate Optimization Algorithm

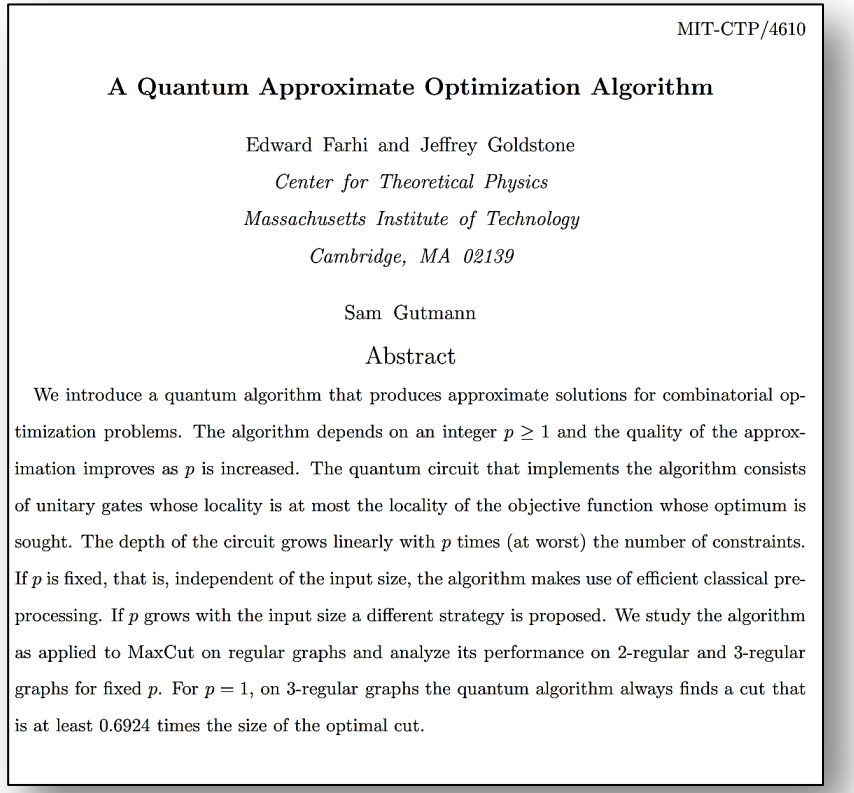
- Gate-based quantum algorithm for QUBO optimization
- Iteratively alternates p times between applying two sets of operators: Mixing and Phase Shifting/Driving
  - Induce entanglement and the objective function
- Requires as many qubits as the size of the problem
- Requires polynomially many gates compared to the problem size
- Is an approximation algorithm:
  - One can theoretically prove that solution to any problem within a certain class using this algorithm will always be in a range (approximation ratio) of the true optimal



Quantum approximate optimization of the long-range Ising model with a trapped-ion quantum simulator
Guido Pagano, Aniruddha Bapat, Patrick Becker, Katherine S. Collins, Arinjoy De, Paul W. Hess, Harvey B. Kaplan, Antonis Kyprianidis, Wen Lin Tan, Christopher Baldwin, Lucas T. Brady, Abhinav Deshpande, Fangli Liu, Stephen Jordan, Alexey V. Gorshkov, Christopher Monroe
Proceedings of the National Academy of Sciences Oct 2020, 117 (41) 25396-25401; DOI: 10.1073/pnas.2006373117

- For MAXCUT of regular 3-degree graphs QAOA with p=1 has approximation ratio of 0.6942 vs. 2/3 of random guessing.
- For a satisfiability problem E3Lin2, QAOA with p=1 gave the best approximation ratio at the point.

Origins of the QAOA



MIT-CTP/4610

A Quantum Approximate Optimization Algorithm

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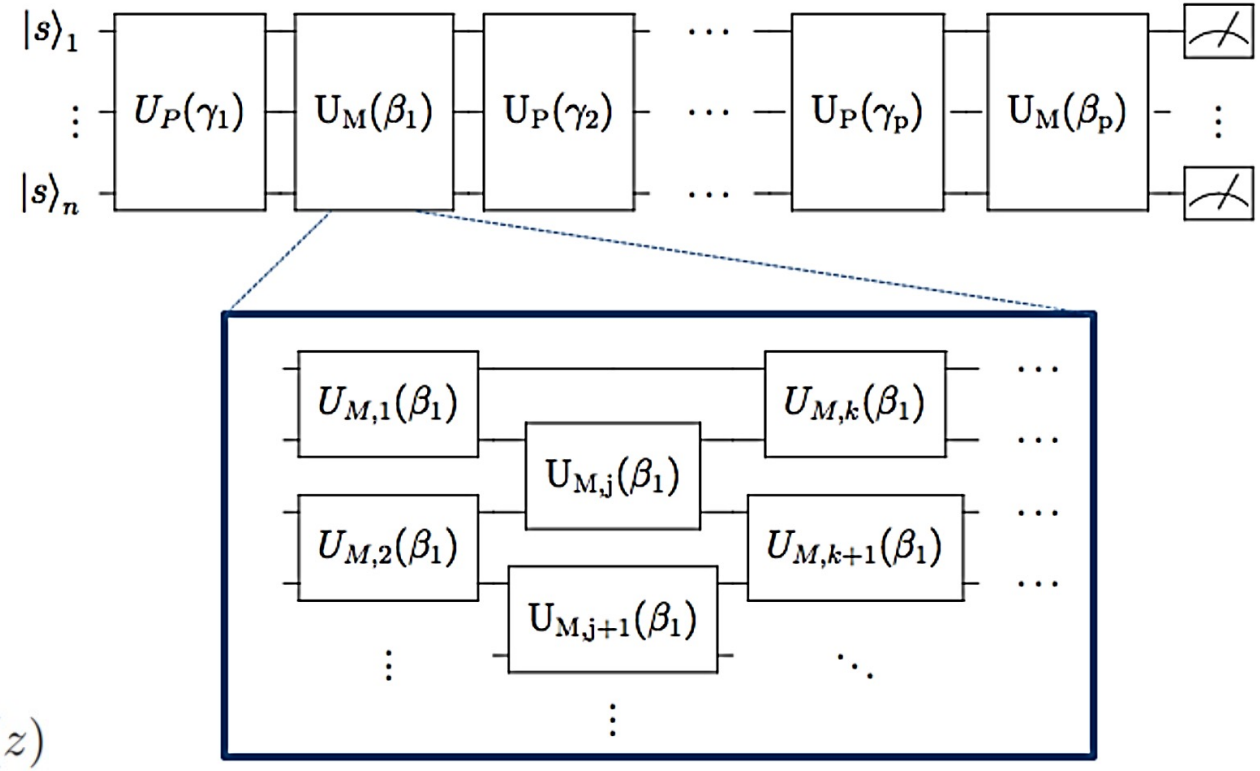
Abstract

We introduce a quantum algorithm that produces approximate solutions for combinatorial optimization problems. The algorithm depends on an integer $p \geq 1$ and the quality of the approximation improves as p is increased. The quantum circuit that implements the algorithm consists of unitary gates whose locality is at most the locality of the objective function whose optimum is sought. The depth of the circuit grows linearly with p times (at worst) the number of constraints. If p is fixed, that is, independent of the input size, the algorithm makes use of efficient classical preprocessing. If p grows with the input size a different strategy is proposed. We study the algorithm as applied to MaxCut on regular graphs and analyze its performance on 2-regular and 3-regular graphs for fixed p. For $p = 1$, on 3-regular graphs the quantum algorithm always finds a cut that is at least 0.6924 times the size of the optimal cut.

$$|\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) \, |s\rangle$$

$$Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) = U_{\mathrm{M}}(\beta_p) U_{\mathrm{P}}(\gamma_p) \cdots U_{\mathrm{M}}(\beta_1) U_{\mathrm{P}}(\gamma_1)$$



$$F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \langle \boldsymbol{\gamma}, \boldsymbol{\beta} | \, C \, | \boldsymbol{\gamma}, \boldsymbol{\beta} \rangle$$

$$M_p = \max_{\boldsymbol{\gamma}, \boldsymbol{\beta}} F_p(\boldsymbol{\gamma}, \boldsymbol{\beta})$$

$$M_p \geq M_{p-1}$$

$$\lim_{p \to \infty} M_p = \max_z C(z)$$

QAOA

1. Design a binary optimization classical Hamiltonian **("phase separation")**
2. Design a unitary operator that can connect and allow jumps between different states **("mixing")**
3. Prepare a QAOA state for some parameters

$$|\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) \, |s\rangle$$

$$Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) = U_{\mathrm{M}}(\beta_p) U_{\mathrm{P}}(\gamma_p) \cdots U_{\mathrm{M}}(\beta_1) U_{\mathrm{P}}(\gamma_1)$$

4. Measure the state in the computational value and compute the exp. value of C(z)

$$F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \langle \boldsymbol{\gamma}, \boldsymbol{\beta} | \, C \, | \boldsymbol{\gamma}, \boldsymbol{\beta} \rangle \qquad M_p \geq M_{p-1}$$

$$M_p = \max_{\boldsymbol{\gamma}, \boldsymbol{\beta}} F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) \qquad \lim_{p \to \infty} M_p = \max_z C(z)$$

5. Change the parameters if they are not proven optimal and repeat 3-4

Vanilla QAOA

$$O_{\text{QUBO}}(q) = \sum_{i=1}^{N} a_i q_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} b_{ij} q_i q_j$$

Associate one qubit to each q_i

Initialize the registers in a superposition of all possible bitstring

$$|\psi\rangle_{in} = \left(2^{N/2}\right)^{-1} \sum_s |s\rangle$$

Assign to each superposed solution a phase proportional (arbitrary parameter γ_1) to its objective function value

$$|\psi\rangle_{ps(1)} = \left(2^{N/2}\right)^{-1} \sum_s e^{i\gamma_1 E_s} |s\rangle$$

Mix the amplitudes by a transverse field rotation $\exp(i\beta X)$ on each qubit (arbitrary parameter)

$$|\psi\rangle_{mix(1)} = \left(2^{N/2}\right)^{-1} \sum_s \mathrm{B}_{1s}(\beta_1, \gamma_1) e^{i\Gamma_{1s}(\beta_1,\gamma_1)} |s\rangle$$

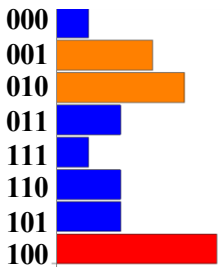
Phase separate again with new γ_2

$$|\psi\rangle_{ps(2)} = \left(2^{N/2}\right)^{-1} \sum_s \mathrm{B}_{1s}(\beta_1, \gamma_1) e^{i(\Gamma_{1s}(\beta_1,\gamma_1) + \gamma_2 E_s)} |s\rangle$$

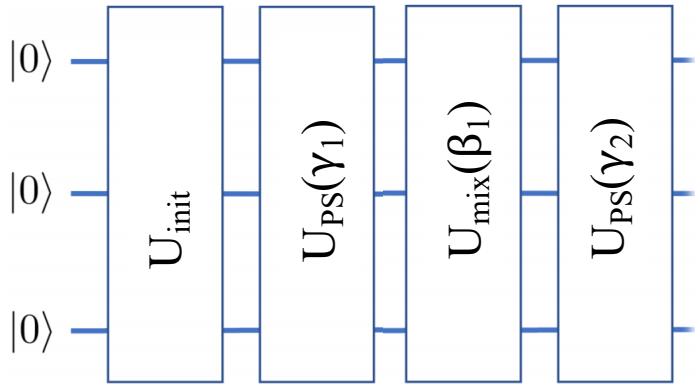
$$|\psi\rangle_{mix(2)} = \left(2^{N/2}\right)^{-1} \sum_s \mathrm{B}_{2s}(\beta_1, \gamma_1, \beta_2, \gamma_2) e^{i(\Gamma_{2s}(\beta_1,\gamma_1,\beta_2,\gamma_2))} |s\rangle$$

After having repeated the algorithm p times do measure in the computational base the expectation value of the objective function

$$\langle\psi|\mathrm{O}|\psi\rangle_{out} = \sum_s \mathrm{O}_s |\mathrm{B}_{ps}|^2$$



Quantum Approximate Optimization Algorithm: Example



Initialization operator

Hadamard Gates

$$|\psi\rangle_{in} = \frac{1}{\sqrt{2^N}} \sum_{n=1}^{2^N} |\text{solution(n)}\rangle$$
$$= \left(2^{N/2}\right)^{-1} \sum_s |s\rangle$$

Phase separation operator dependent on a parameter γ_1

$$\underbrace{\exp(i\beta Z_1 Z_2)}|s_1 s_2\rangle = e^{i\gamma_1 s_1 s_2}|s_1 s_2\rangle$$

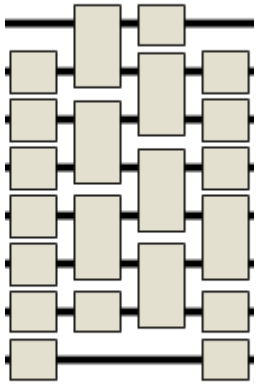
Logical 2-qubit gate representing the Ising interaction

$$|\psi\rangle_{ps(1)} = \frac{1}{\sqrt{2^N}} \sum_{n=1}^{2^N} e^{iE_n}|solution(n)\rangle$$

Mix the amplitudes by a transverse field rotation $\exp(i\beta X)$ on each qubit (arbitrary parameter)

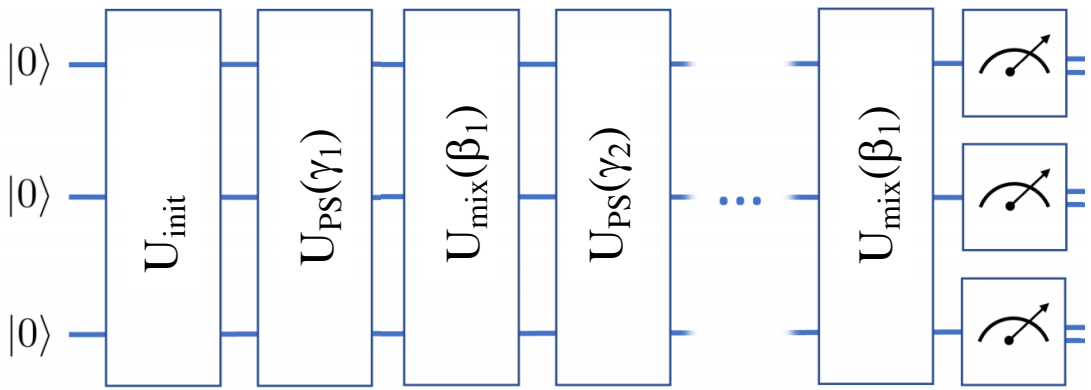
$$|\psi\rangle_{mix(1)}$$
$$= \left(2^{N/2}\right)^{-1} \sum_s B_{1s}(\beta_1, \gamma_1) e^{i\Gamma_{1s}(\beta_1,\gamma_1)}|s\rangle$$

Now if you measure, the probability of a bitstring depends both on γ and β in a non-linear way.



You need to schedule the gates for every term of the objective function !

Quantum Approximate Optimization Algorithm: Example



Now if you measure, the probability of a bitstring depends both on γ and β in a non-linear way.
It is exponentially difficult to predict or simulate the probability $\left|\mathrm{B}_{2s}(\beta_1,\gamma_1,\beta_2,\gamma_2,\dots,\beta_p,\gamma_p)\right|^2$ to find the optimal unknown solution s^*

$$|\psi\rangle_{\mathrm{QAOA}(p)} = \left(2^{N/2}\right)^{-1}\sum_s \mathrm{B}_{2s}(\beta_1,\gamma_1,\beta_2,\gamma_2,\dots,\beta_p,\gamma_p)e^{i\Gamma_{1s}(\beta_1,\gamma_1,\beta_2,\gamma_2,\dots,\beta_p,\gamma_p)}|s\rangle$$

For $p \to \infty$ you can map this evolution to AQC; discrete becomes continuous; so, you know how to do it.
For finite p there is currently not a lot of guidance, big sector of research.
The search over the parameter space γ and β is done heuristically (e.g., Gradient descent)

QAOA for Constrained Optimization Problems

QAOA for Constrained Combinatorial Optimization

** Stay in the computational subspace!*

Associate one qubit to each q_i

Initialize the registers with a candidate solution found through genetic algorithm or greedy search

$|\psi\rangle_{in}=|011010101100\rangle$

Mix the system by generating a superposition of the initial solution with all possible others (arbitrary parameter)

$|\psi\rangle_{mix}=\alpha|011010101100\rangle+\sum_k \beta_k|\phi_k\rangle$

Mix with new β^*

Add phases again with new γ

Assign to each superposed solution a phase proportional (arbitrary parameter) to its objective function value

$|\psi\rangle_{mix}=\alpha e^{i\gamma E_{in}}|011010101100\rangle + \sum_k \beta_k e^{i\gamma E_k}|\phi_k\rangle$

DIFFICULT

Only the logical subspace

VS

$|\psi\rangle_{mix}=\sum_s \beta_s|s\rangle$

All 2^N bitstrings

The Problem of Hard Constraints

$$O_{\text{QUBO}}(q) = \sum_{i=1}^{N} a_i q_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} b_{ij} q_i q_j$$

$$\boxed{\sum_i q_i = k} \xrightarrow{\text{Penalty Function}} c\left(\sum_i q_i - k\right)^2$$

Difficult to scale, does not guarantee results, hardness is large softness

What you would want is to start from a classical bitstring, and then be able to "mix it" coherently in the subspace where the constraint is satisfied

Enforcing the same number of bits=1 is the same as doing two spin-flips

$$|001\rangle \xrightarrow{XY(2,3)} a|001\rangle + b|010\rangle \xrightarrow{XY(2,3)} a'|001\rangle + b'|010\rangle + c'|100\rangle$$

$$\mathrm{XY}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\frac{\theta}{2} & i\sin\frac{\theta}{2} & 0 \\ 0 & i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Possible solution for these constraints: *XY*-Mixers.

QAOA Applications

- Maximum Cut
- Max-SAT, Min-SAT, NAE-SAT
- Set Splitting
- MaxE3LIN2
- Max-ColorableSubgraph
- Graph Partitioning
- Maximum Bisection
- Max Vertex k-Cover
- MaxIndependentSet
- MaxClique
- MinVertexCover
- MaxSetPacking
- MinSetCover
- TSP
- SMS with various metrics and constraints
- …

Objective Function: Soft Constraints
Feasible States: Hard Constraints

Quantum Approximate Optimization with Hard and Soft Constraints

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ABSTRACT

Challenging computational problems arising in the practical world are frequently tackled by heuristic algorithms. Small universal quantum computers will emerge in the next year or two, enabling a substantial broadening of the types of quantum heuristics that can be investigated beyond quantum annealing. The immediate question is: what experiments should we prioritize that will give us insight into quantum heuristics? One leading candidate is the quantum approximate optimization algorithm (QAOA) metaheuristic. In this work, we provide a framework for designing QAOA circuits for a variety of combinatorial optimization problems with both hard constraints that must be met and soft constraints whose violation we wish to minimize. We work through a number of examples, and discuss design principles.

CCS CONCEPTS

• **Mathematics of computing** → **Approximation algorithms**; • **Hardware** → **Emerging technologies**; **Quantum computation**; • **Theory of computation** → *Quantum computation theory*; *Mathematical optimization*;

advantage, and if so, how to design quantum algorithms that realize such advantages. Today, challenging computational problems arising in the practical world are frequently tackled by heuristic algorithms, which by definition have not been analytically proven to be the best approach, or even proven analytically to outperform the best approach of the previous year. Rather, these algorithms are empirically shown to be effective, by running them on characteristic sets of problems, or demonstrating their effectiveness in practical applications. As prototype quantum hardware emerges, this approach to algorithm design becomes available for the evaluation of quantum heuristic algorithms.

For several years now, special-purpose quantum hardware has been used to explore one quantum heuristic algorithm, quantum annealing. Emerging gate-model processors, which are universal in that, once scaled up, they can run any quantum algorithm, will enable investigation of a much broader array of quantum heuristics beyond quantum annealing. Within the last year, IBM has made available publicly through the cloud a 5-qubit gate-model chip [13], and announced recently an upgrade to a 17-qubit chip. Likewise, Google [3] and Rigetti Computing [22], anticipate providing processors with 40–100 qubits within a year or two [18]. Many academic

Alternating Operator Ansatz

$$Q_p(\boldsymbol{\beta},\boldsymbol{\gamma}) = U_{\mathrm{M}}(\beta_p)U_{\mathrm{P}}(\gamma_p)\cdots U_{\mathrm{M}}(\beta_1)U_{\mathrm{P}}(\gamma_1)$$

$$|\boldsymbol{\beta},\boldsymbol{\gamma}\rangle = Q_p(\boldsymbol{\beta},\boldsymbol{\gamma})\,|s\rangle$$

$$\boxed{e^{-i\beta H_{\mathrm{M}}}}$$

$$\boxed{e^{-i\gamma H_{\mathrm{P}}}}$$

Some initial state respecting:

- It is a superposition of several solutions in the feasible subspace
- It can be prepared efficiently

Some unitary respecting:

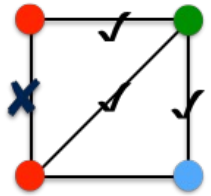
- Preserve the feasible subspace
- Provide all-to-all nonzero transitions between all feasible states
- Non-necessarily time evolution of a local Hamiltonian

Some unitary respecting:

- Is diagonal in the computational basis
- The spectrum of H_P encodes the objective function

$$H_f\,|\mathbf{x}\rangle = f(\mathbf{x})\,|\mathbf{x}\rangle$$

Graph Coloring

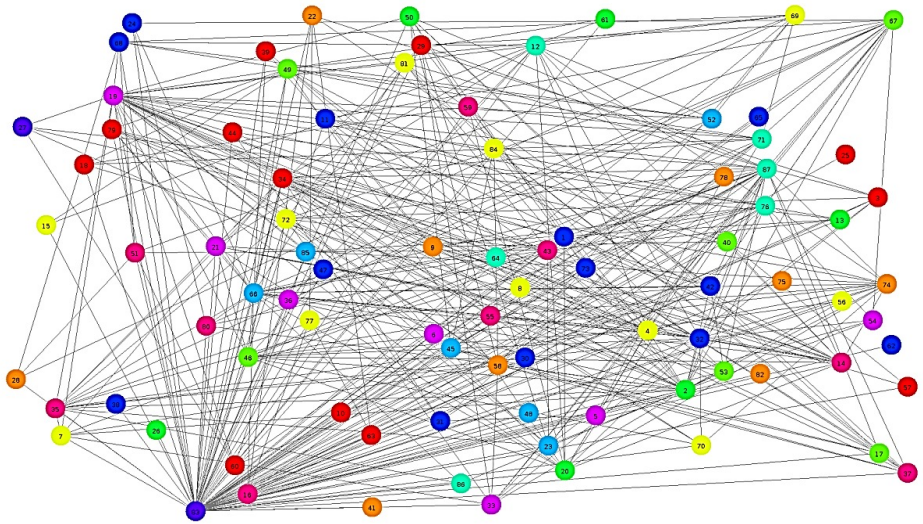


$X_{ic}=1$ if node **i** is colored by color **c**

$X_{ic}=0$ otherwise

$\sum_{(i,j)\epsilon E} X_{ic}\, X_{jc}$ counts the conflicts (soft constraint)

$\sum_c X_{ic}=1$ enforces a unique coloring (hard constraint)



If both $|X_{ic}\rangle$ and $|X_{jc}\rangle$ are $|1\rangle$ then introduce a phase (phase separation angle)

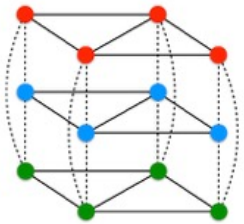
$$\mathrm{CPHASE}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix}$$

$$|001\rangle \xrightarrow{XY(2,3)} a\,|001\rangle + b\,|010\rangle \xrightarrow{XY(2,3)} a'\,|001\rangle + b'\,|010\rangle + c'\,|010\rangle$$

$$\mathrm{XY}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\frac{\theta}{2} & i\sin\frac{\theta}{2} & 0 \\ 0 & i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$[X_1X_2 + Y_1Y_2, Z_1 + Z_2] = 0$$

Work in a coherent superposition of hamming weight 1 states (mixing in the feasibility subspace)

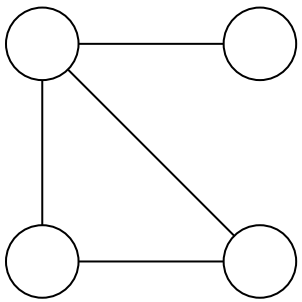


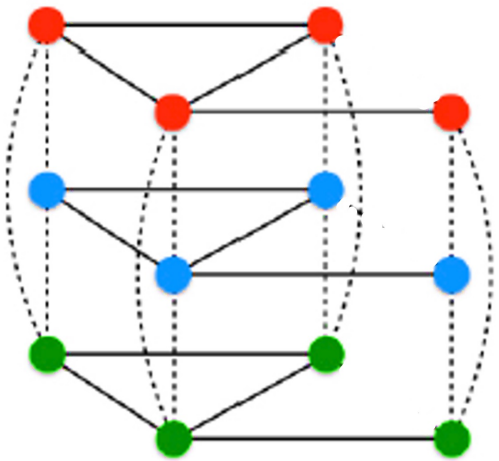
Alternating Operator Ansatz

Node u is colored by c

$X_{u,c}=1$

$$m - \sum_{\{u,v\}\in E} \sum_{a=1}^{k} x_{u,a} x_{v,a}$$





Phase Separator (QUBO objective function)

$$H'_{\mathrm{P}} = \frac{4-\kappa}{4} mI + \frac{1}{4} \sum_{\{u,v\}\in E} \sum_{a=1}^{\kappa} (Z_{u,a} + Z_{v,a} - Z_{u,a} Z_{v,a})$$

Initial state:

$$|W\rangle_v = \frac{1}{\sqrt{k}} (|100\cdots0\rangle + |010\cdots0\rangle + |0\cdots01\rangle)$$

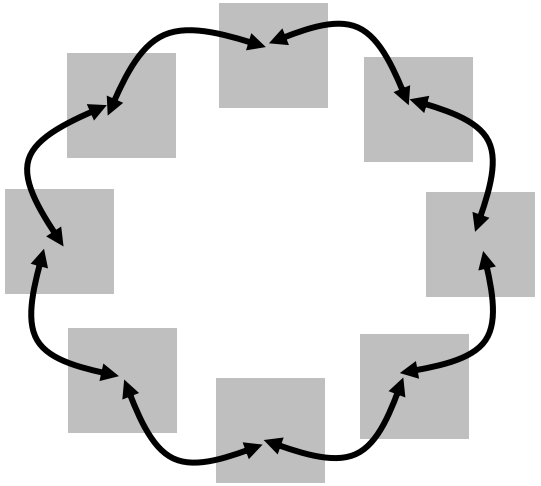
- *Babbush (2017)*
- *Verstraete (2009)*
- *Wang (2009)*
- *Childs (2002)*
- ...

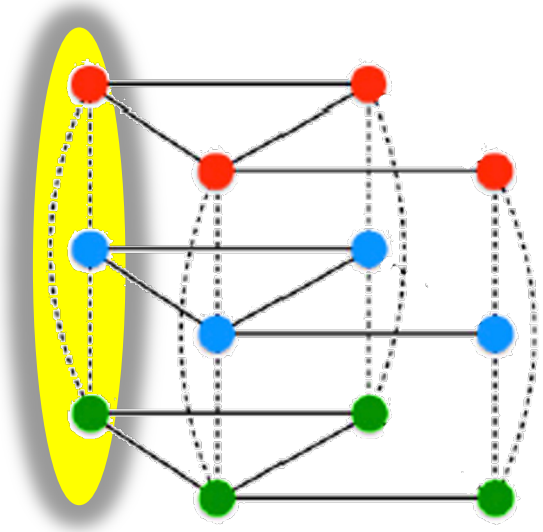
Engineering Mixing Operators

$$H_{\text{ring}}^{(\text{enc})} = \sum_{a}^{d} (X_a X_{a+1} + Y_a Y_{a+1})$$

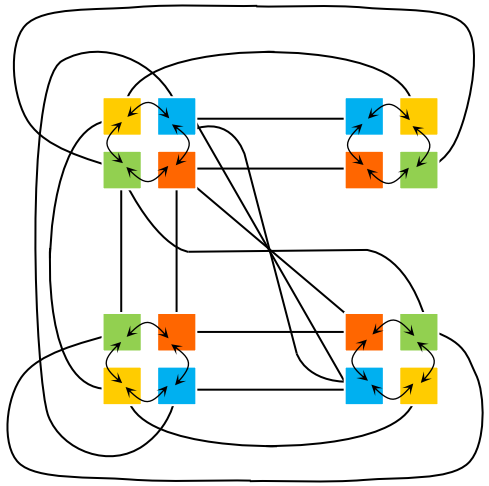
$\exp(iH_{\text{ring}})$ is difficult to implement

Respects the Hamming Weight constraint





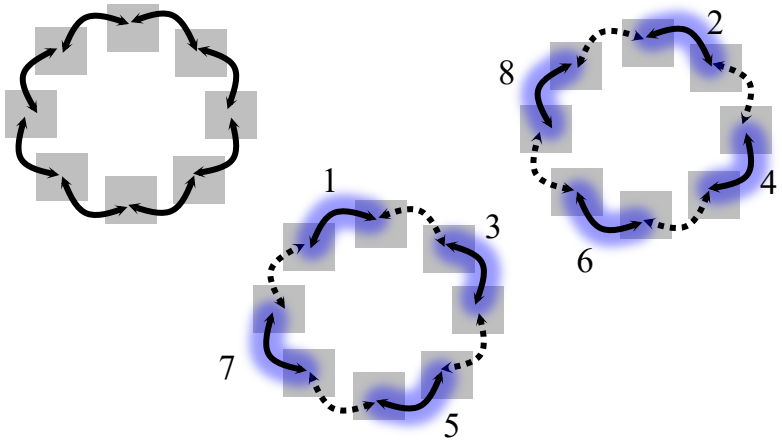
3-coloring



4-coloring

Advanced: Desing Freedom and Implementation Tradeoffs

You can't execute two gates at the same time sharing the same qubit!



$$H_{\text{ring}}^{(\text{enc})} = \sum_{a}^{d} (X_a X_{a+1} + Y_a Y_{a+1})$$

Respects the Hamming Weight constraint

$\exp(iH_{\text{ring}})$ is difficult to implement

$$U_{\text{M}} = \prod_{v=1}^{n} U_{v,\text{parity}}^{(\text{enc})}$$

$\prod_{a \in \text{parity}} \text{Exp}(iX_a X_{a+1} + Y_a Y_{a+1})$

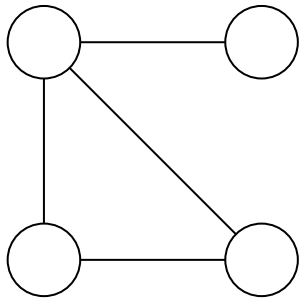
$$U_M = \underbrace{[U_1 U_3 U_5 U_7]\ [U_2 U_4 U_6 U_8]}\ [U_1 U_3 U_5 U_7]\ [U_2 U_4 U_6 U_8] \ldots$$

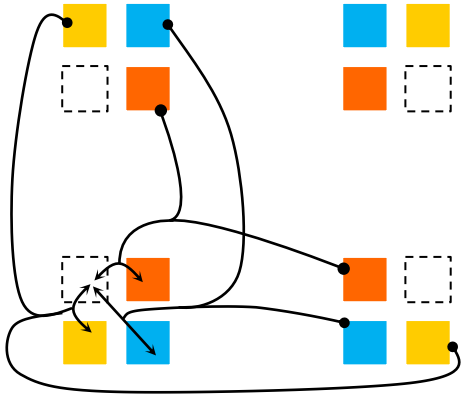
This couples only distance 2;
has to be repeated k/2 times

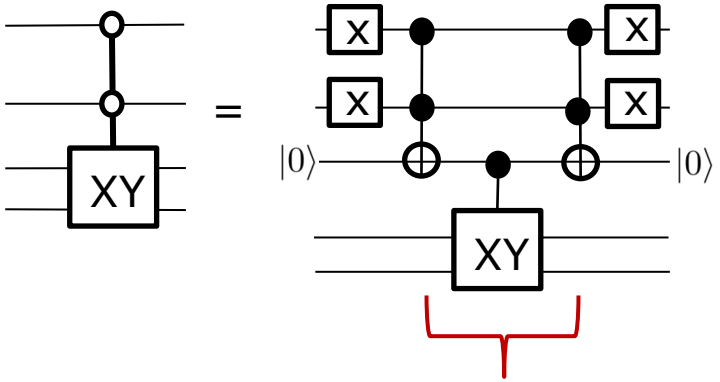
All these 2-qubit $k^2/2$ gates need to be scheduled

Other Mixers (controlled XY)

Finding the largest induced subgraph colorable by k colors







Still needs to be compiled to 2 qubit gates

All these gates need to be scheduled

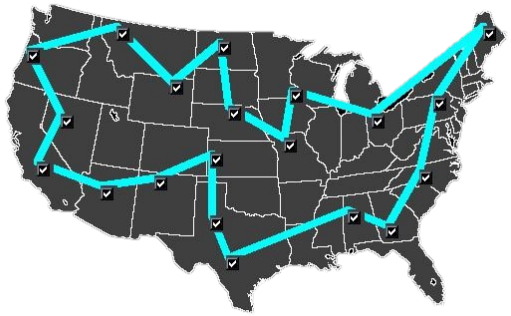
Node u is colored by c or uncolored (c=0)

$X_{u,c}=1$

$$C = m - \sum_{v} x_{v,0} \rightarrow H_C = \frac{1}{2}\sum_{v} Z_{v,0}$$

Mixers Navigation&Scheduling

In **traveling salesman** encoding



$X_{vj}=1$ if city v is visited as j^{th}

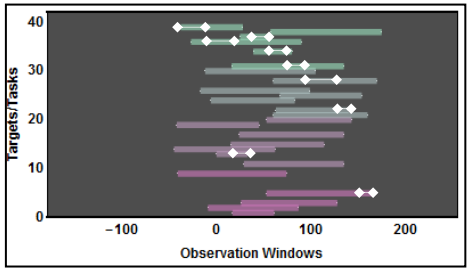
$$\sum_{\{u,v\}\in E} d_{u,v} \sum_{j=1}^{n} \left(x_{u,j}x_{v,j+1} + x_{v,j}x_{u,j+1}\right)$$

$$H^{(\mathrm{enc})}_{\mathrm{PS},\{i,j\},\{u,v\}} = S^{+}_{u,i}S^{+}_{v,j}S^{-}_{u,j}S^{-}_{v,i} + S^{-}_{u,i}S^{-}_{v,j}S^{+}_{u,j}S^{+}_{v,i},$$

(partitioned using edge coloring and parity $\approx (n-1)n^2/4$ mixers)

(needs to be repeated n(n-1)/2 times for all-to-all)

In **single machine scheduling**



$X_{jt}=1$ if job j starts at time t

$$C = \sum_{j} w_j \sum_{(d_j-p_j)<t<h} x_{j,t}(t + p_j - d_j)$$

$$H^{(\mathrm{enc})}_{\mathrm{TS},t,\{i,j\}} = S^{+}_{i,t+p_j}S^{+}_{j,t}S^{-}_{i,t}S^{-}_{j,t+p_i} + S^{+}_{i,t}S^{+}_{j,t+p_i}S^{-}_{i,t+p_j}S^{-}_{j,t},$$

(But if we add release dates then we need controls on the no-overlap constraint)

Zoology of Ansatze

(See Hadfield et al 2018 – «Quantum Alternating Operator Ansatz»)

Bitflip mixers
- Maximum Cut
- Max-SAT, Min-SAT, NAE-SAT
- Set Splitting
- MaxE3LIN2

...

XY mixers
- Max-ColorableSubgraph
- Graph Partitioning
- Maximum Bisection
- Max Vertex k-Cover

...

Controlled Bitflip mixers
- MaxIndependentSet
- MaxClique
- MinVertexCover
- MaxSetPacking
- MinSetCover

...

Controlled XY mixers
- Max-k-ColorableInducedSubgraph
- MinGraphColoring
- MinCliqueCover

...

Permutation mixers
- TSP
- SMS with various metrics and constraints

...

From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz

Stuart Hadfield*, Zhihui Wang+,**, Bryan O'Gorman+,†,‡, Eleanor G. Rieffel+, Davide Venturelli+,**, Rupak Biswas+

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+ Quantum Artificial Intelligence Lab., NASA Ames Research Center, Moffett Field, CA
** USRA Research Institute for Advanced Computer Science (RIACS), Mountain View, CA
† Stinger Ghaffarian Technologies, Inc., Greenbelt, MD
‡ Berkeley Quantum Information and Computation Center and Departments of Chemistry and Computer Science, University of California, Berkeley, CA

September 12, 2017

The next few years will be exciting as prototype universal quantum processors emerge, enabling implementation of a wider variety of algorithms. Of particular interest are quantum heuristics, which require experimentation on quantum hardware for their evaluation, and which have the potential to significantly expand the breadth of applications for which quantum computers have an established advantage. A leading candidate is Farhi et al.'s Quantum Approximate Optimization Algorithm, which alternates between applying a cost-function-based Hamiltonian and a mixing Hamiltonian. Here, we extend this framework to allow alternation between more general families of operators. The essence of this extension, the Quantum Alternating Operator Ansatz, is the consideration of general parameterized families of unitaries rather than only those corresponding to the time-evolution under a fixed local Hamiltonian for a time specified by the parameter. This ansatz supports the representation of a larger, and potentially more useful, set of states than the original formulation, with potential long-term impact on a broad array of application areas.

Brief intro to NISQ Era Quantum Computers available today

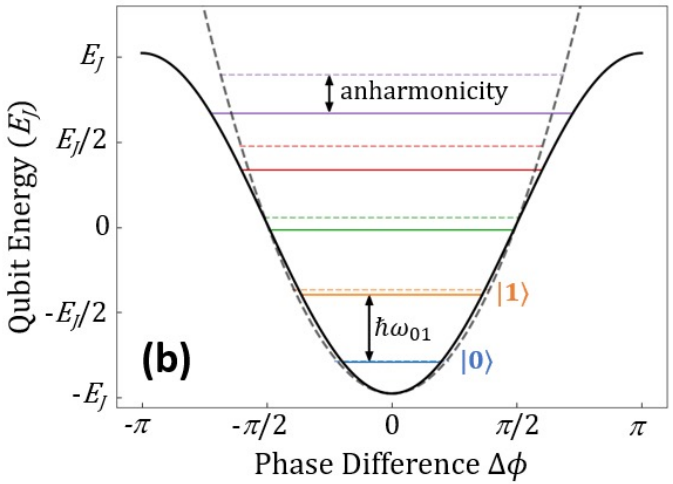
Superconducting: Transmons

A Quantum Engineer's Guide to Superconducting Qubits
P. Krantz[1,2,†], M. Kjaergaard[1], F. Yan[1], T.P. Orlando[1], S. Gustavsson[1], and W. D. Oliver[1,3,‡]

https://arxiv.org/pdf/1904.06560.pdf

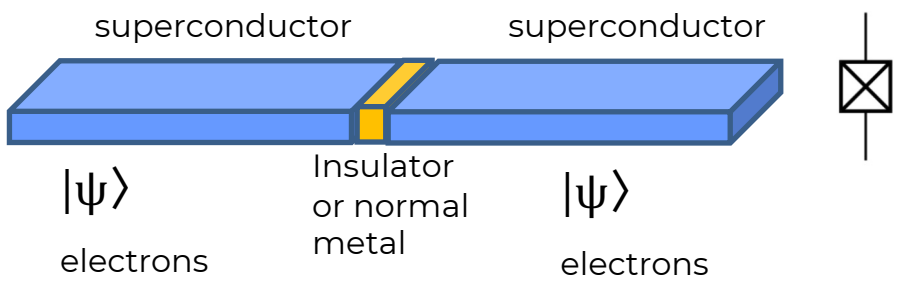
Tutorial: Gate-based superconducting quantum computing
Sangil Kwon,[1,a)] Akiyoshi Tomonaga,[1,2] Gopika Lakshmi Bhai,[1,2] Simon J. Devitt,[3] and Jaw-Shen Tsai[1,2]

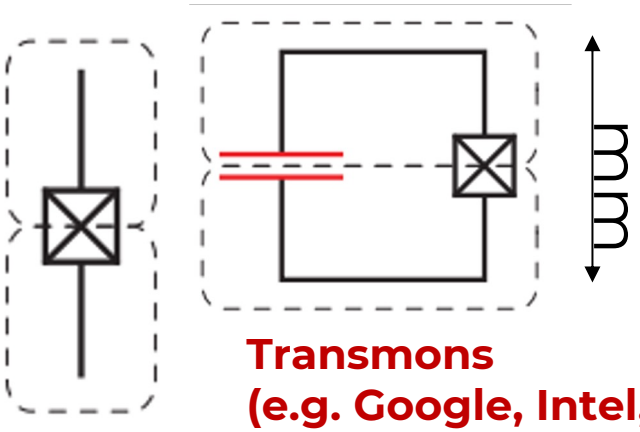
https://arxiv.org/pdf/2009.08021.pdf



If two superconductors are separated by a thin barrier, their wavefunction communicates and creates a tunneling current with non-linear properties

(Josephson Effect; Josephson Junctions – Phys. Lett. 1. 251 - 1962)





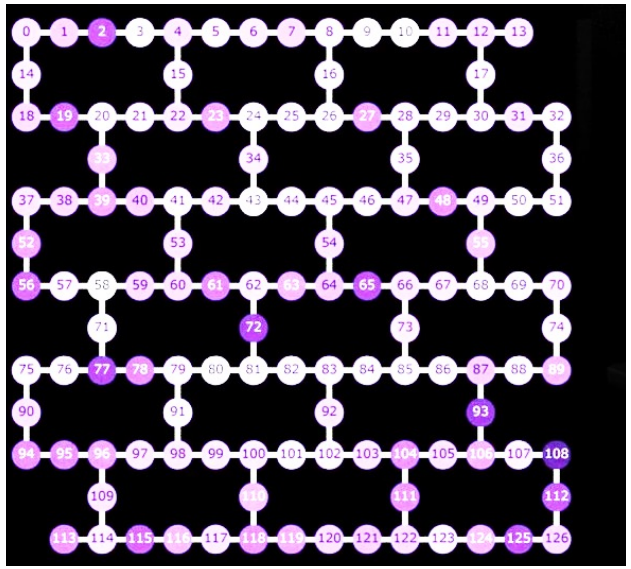
Transmons (e.g. Google, Intel, IBM, Rigetti)

LEADING QUBITS DESIGN

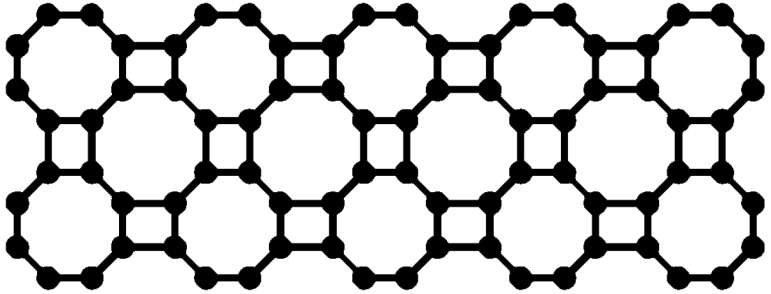
- High quality factor
- Ability to be coupled to other transmons.
- Absorb/Emit in microwave region (Ghz)

Superconducting: Vendors

Current: 127 IBM Eagle
Roadmap: 433 (2022); 1121 (2023)
Basis gates: CX, ID, RZ, SX, X



Current: 80 M-1
Roadmap: 336 (2023) 1000+ (2025)
Basis gates: RX, RY, RZ, CPHASE, XY

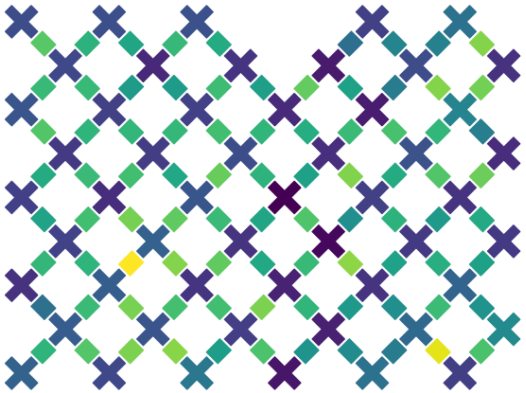


CPHASE

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix}$$

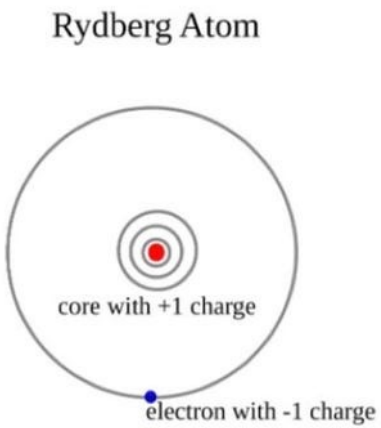
$$\mathrm{XY}(\beta,\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\frac{\theta}{2}) & i\sin(\frac{\theta}{2})e^{i\beta} & 0 \\ 0 & i\sin(\frac{\theta}{2})e^{-i\beta} & \cos(\frac{\theta}{2}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

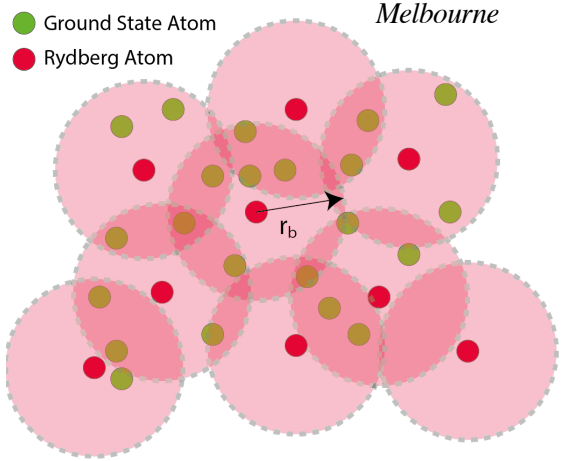
Current: 72(53)
Roadmap: 1 logical qubit! Undisclosed
Basis gates: RX, RY, RZ, fSim



$$\mathrm{fSim}(\theta,\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & -i\sin\theta & 0 \\ 0 & -i\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{pmatrix}$$

Neutral Atoms: analog simulators





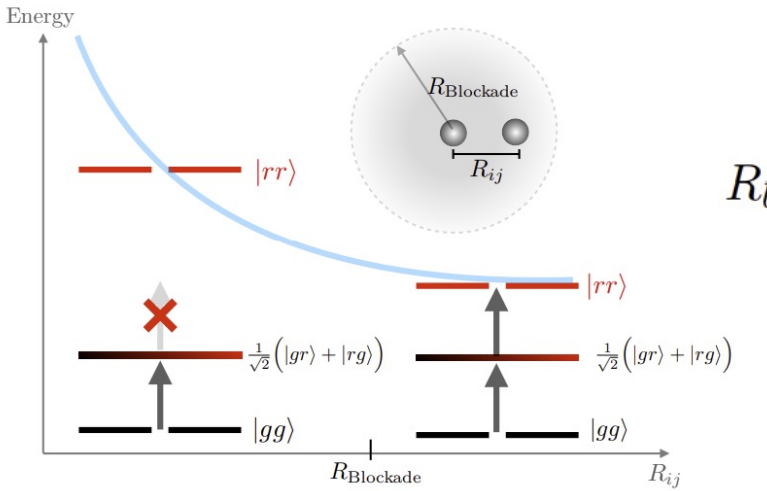
From: *University of Melbourne*

$$\mathcal{H}(t) = \sum_i \left(\frac{\hbar\Omega(t)}{2}\sigma_i^x - \hbar\delta(t)\hat{n}_i + \sum_{j<i} \frac{C_6}{(R_{ij})^6}\hat{n}_i\hat{n}_j \right)$$

$$\hat{n}_i = (1 + \sigma_i^z)/2$$ Ising Hamiltonian

$$\mathcal{H}_{int} = 2\sum_{i\neq j} \frac{C_3}{R_{ij}^3}\left(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y\right)$$ XY Hamiltonian

Atoms that allow high-orbital occupation (Rydberg), interacting through Van-Der-Waals electrostatic interaction, are effectively implementing “Ising” or “XY” between two computational states.



$$R_b = \left(\frac{C_6}{\hbar\Omega}\right)^{1/6}$$

Pulser: An open-source package for the design of pulse sequences in programmable neutral-atom arrays

Henrique Silvério[1,*], Sebastián Grijalva[1,*], Constantin Dalyac[1], Lucas Leclerc[1], Peter J. Karalekas[2], Nathan Shammah[2], Mourad Beji[1], Louis-Paul Henry[1], and Loïc Henriet[1]

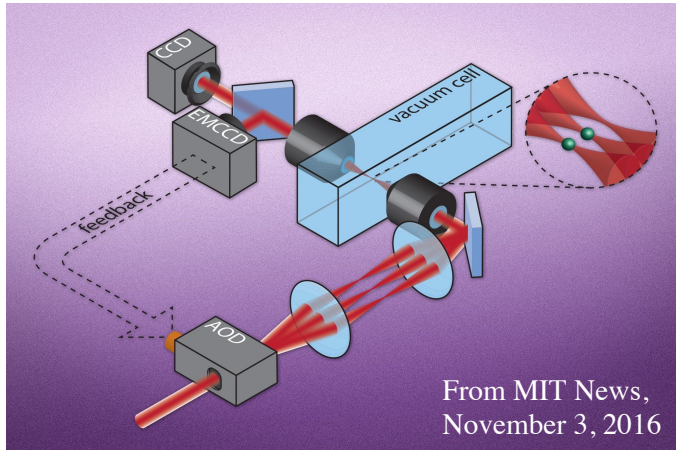
Unitary Fund

Electrical & Computer ENGINEERING

TEPPER

USRA Universities Space Research Association

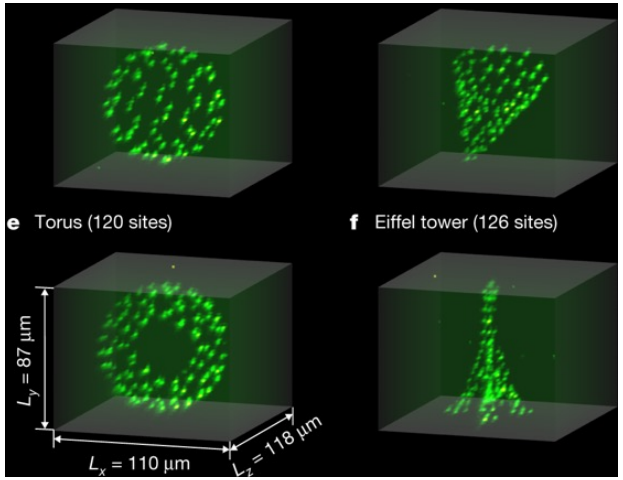
Neutral Atoms: processor architectures, vendors and results



Current technology allows to place atoms in arbitrary 3D structures – but the laser excitation triggering dipole interaction is still "global" on a large part of the processor.

Current: 256 quantum analog (rubidium) soon on AWS
Roadmap: 1024 QPU by 2024

Current:: 100 qubits (rubidium) available now on CINECA, 300 qubit in dev (Microsoft Azure)
Roadmap: 1000 qubits in 2023



Note: Coldquanta and Atom Computing are focusing on digital quantum computing with Rydberg (cesius, strontium) – no product yet.

Barredo, D., Lienhard, V., de Léséleuc, S., Lahaye, T. & Browaeys, A. Nature 561, 79–82 (2018)

Ion Trap Processors: 1D dipole-dipole architecture

IONQ

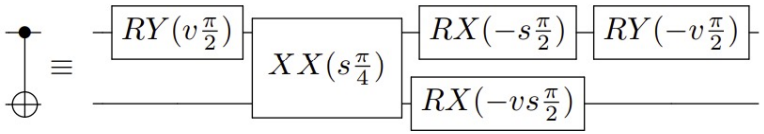
Native Gates:

$$GPI(\phi) = \begin{bmatrix} 0 & e^{-i\phi} \\ e^{-i\phi} & 0 \end{bmatrix}$$

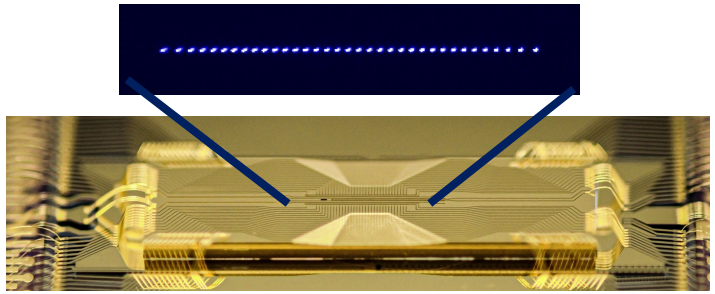
$$GPI2(\phi) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -ie^{-i\phi} \\ -ie^{i\phi} & 1 \end{bmatrix}$$

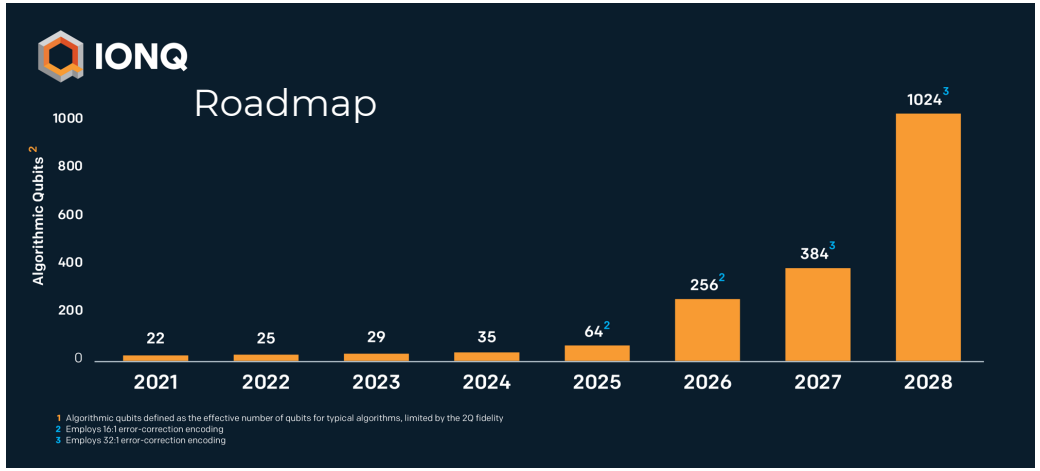
$$Virtual\ Z(\theta) = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

$$XX(\chi) = \begin{pmatrix} \cos(\chi) & 0 & 0 & -i\sin(\chi) \\ 0 & \cos(\chi) & -i\sin(\chi) & 0 \\ 0 & -i\sin(\chi) & \cos(\chi) & 0 \\ -i\sin(\chi) & 0 & 0 & \cos(\chi) \end{pmatrix}$$



- Linear trap holds the ions (ytterbium) in place via oscillating fields (paul trap) – only 1D, currently 32 (max ≈100 ions) separated few microns.
- Lasers displace atoms ≈nm induce dipole-dipole interaction in arbitrary pairs of qubits. Gate time 10-100 us; Fidelity ≈99+% - full connectivity but parallelization is difficult from the quantum control point of view.



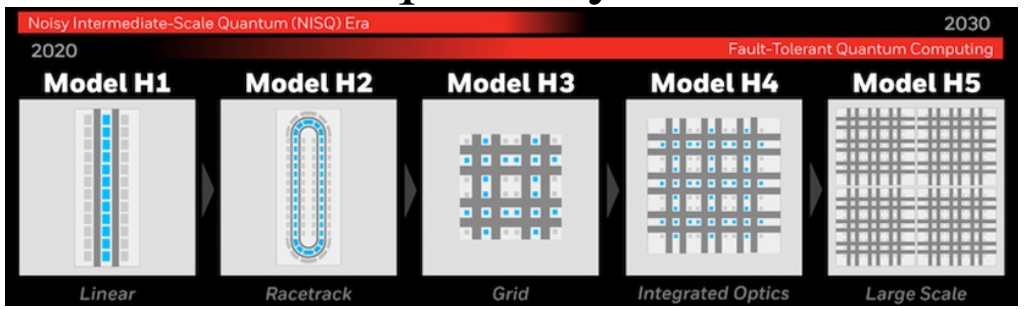


Ion Trap Processors: Quantum Charge Coupled Device (QCCD)

QUANTINUUM

Same as ion-Q but the traps are designed to have regions of movement of ions, and regions of interactions. Motional mode are not exploited except by a small number of ions when closeby with the others separated.

≈512 qubits by 2025



$$U_{1q}(\theta,\varphi) = e^{-i\,(\cos\varphi\hat{X}+\sin\varphi\hat{Y})\,\theta/2} = \begin{pmatrix} \cos\frac{\theta}{2} & -ie^{-i\varphi}\sin\frac{\theta}{2} \\ -ie^{i\varphi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

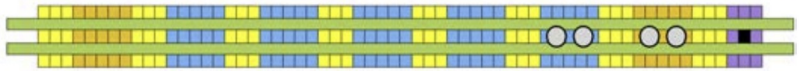
Native Gates

$$R_z(\lambda) = e^{-i\,\hat{Z}\,\lambda/2} = \begin{pmatrix} e^{-i\,\lambda/2} & 0 \\ 0 & e^{i\,\lambda/2} \end{pmatrix}$$

$$ZZ() = e^{-i\,\pi/4\hat{Z}\otimes\hat{Z}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Operation	Duration(μs)
Qubit initialization	10
Qubit measurement (high-fidelity)	120
Qubit measurement (low crosstalk)	60
Cooling stage 1 (Doppler)	550
Cooling stage 2 (Axial and Radial SB)	850
Cooling stage 3 (Axial SB)	650
SQ $\pi/2$ time	5
TQ gate	25

System Fundamentals	H1-1			H1-2		
Parameters	**min**	**typ**	**max**	**min**	**typ**	**max**
General						
Qubits		20			12	
Average depth-1 circuit time[1]		28 ms			27 ms	
Connectivity		All-to-all			All-to-all	
Parallel two-qubit operations		5			3	
Errors						
Single-qubit gate infidelity	2×10^{-5}	5×10^{-5}	3×10^{-4}	2×10^{-5}	5×10^{-5}	3×10^{-4}
Two-qubit gate infidelity	2×10^{-3}	3×10^{-3}	5×10^{-3}	2×10^{-3}	3×10^{-3}	5×10^{-3}
State preparation and measurement (SPAM) error	2×10^{-3}	3×10^{-3}	5×10^{-3}	2×10^{-3}	3.5×10^{-3}	6×10^{-3}
Memory error per qubit at average depth-1 circuit	1×10^{-4}	4×10^{-4}	1×10^{-3}	1×10^{-4}	4×10^{-4}	1×10^{-3}
Mid-circuit measurement cross-talk error	5×10^{-5}	1×10^{-4}	5×10^{-4}	5×10^{-5}	1×10^{-4}	5×10^{-4}



Linear Transport (physical shuttling)
SWAP Operation (physical out-of-plane swaps)

Operation	Duration (μs)
Intrazone shift	58
Interzone shift	283
Split/combine	128
Swap	200

QAOA in the “Real World”

The Flexible Design of NISQ Quantum Optimization Algorithms

Vanilla QAOA (Fahri 2014) and the QAOAnsatz (Hadfield 2017) were just the start of the field of modern Quantum Optimization Approaches

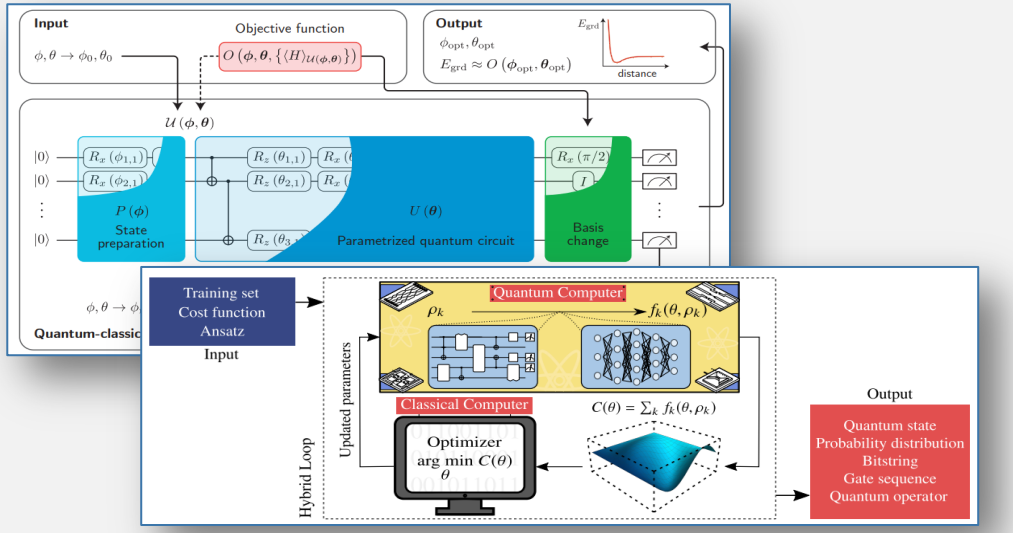
Variations:

- **Incomplete/Approximate:** e.g. mixing of a limited number of variables randomly selected.
- **Adaptive:** e.g. changing the circuit at runtime based on parameter exploration.
- **Unstructured:** e.g. the cost function could be evaluated only by classical hardware and is not in the ansatz, like learning in a neural network.
- **Overparametrized:** e.g. some gates might have offset angles
- **Digital-Analog:** i.e. global pulsing techniques that generate multi-qubit long range interactions.

Recent Review Articles:

Noisy intermediate-scale quantum (NISQ) algorithms
Bharti et al. (Jan 2021) – arXiv:2101.08448

Variational Quantum Algorithms
Cerezo et al. (Dec 2020) – arXiv:2012.09265

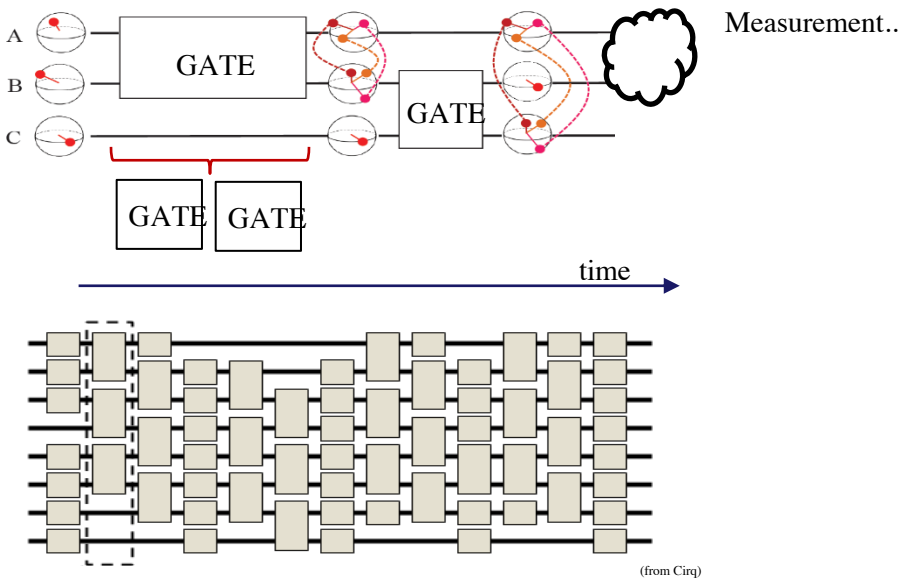


A Circuit View of QAOA algorithms

IDEALIZED QUANTUM CIRCUIT
What is the best way to express the unitary transformation that implements the algorithms?
(you cannot write the matrix)

SYNTHESIS
... in term of the natively implementable gates?

COMPILATION (PARALLELIZATION)
... minimizing the duration of the execution of the circuit?
Or the total infidelity of the computation?

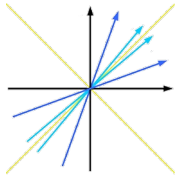


The Gate Synthesis Problem

Barenco et al. (1995)
Kraus, Cirac (2001)
Vatan, Williams (2003)

Quantum Circuits can be composed by single and two-qubit gates of universal set*
CNOT, $R_y(q)$ and $R_z(a)$

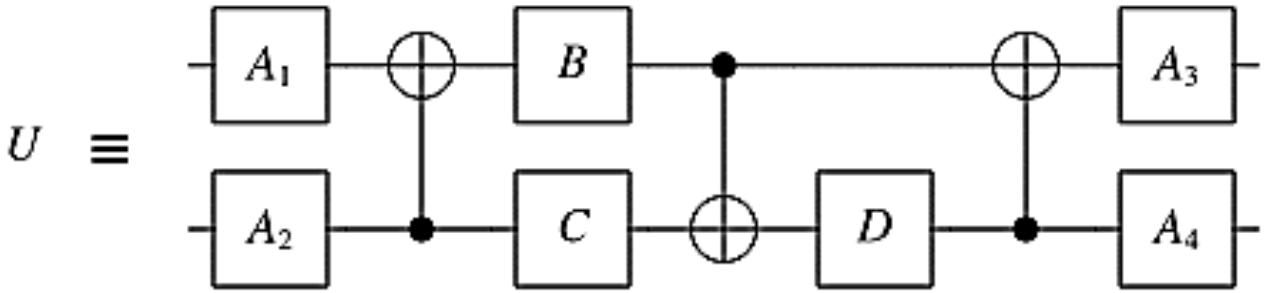
Each single qubit gate can be decomposed by single qubit rotations.
U1= $R_z(a)\ R_y(b)\ R_z(g)\ e^{if}$



Each two qubit gate is reversible and it is representable by a Unitary Matrix.

R_Z gates can be «virtually» compiled.
(McKay 2017 and refs)

* active research to natively support multi-qubit gates



Maximum number of elementary 1-qubit gates: **15**
Maximum number of CNOTs: **3**
Maximum depth assuming R_Y, R_Z and simplifications: **11**

SWAP-Compilation (review)

Performance of algorithms in NISQ will depend on aspects such as gate fidelities, parallelization, idle time, crosstalks..

Different Metrics to optimize correlate to final performance:

- Total Quantum Factor
- Quantum Volume
- Number of Two-Qubit Gates
- **Makespan**

Guerreschi and Park (2018). Two-step approach to scheduling quantum circuits. *arXiv preprint arXiv:1708.00023*.

Khatri, Sumeet, et al. "Quantum assisted quantum compiling." *arXiv preprint arXiv:1807.00800* (2018).

Li, G., Ding, Y., & Xie, Y. (2018). Tackling the Qubit Mapping Problem for NISQ-Era Quantum Devices. *arXiv preprint arXiv:1809.02573 (2018)*.

Oddi, Angelo, and Riccardo Rasconi. "Greedy Randomized Search for Scalable Compilation of Quantum Circuits." *International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*. Springer, Cham, (2018.

…

Example: MaxCut

$S_i = \pm 1$ Defines the cut

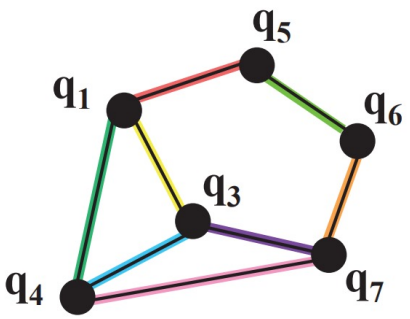
$$U = \frac{1}{2} \sum_{(i,j)\in E} (1 - s_i s_j)$$ Counts the edges in the cut

$\sum_i X_i$ Mixes the two partitions

$U_{PS} = \Pi_{<jk>} Exp(ibZ_j Z_k)$

$U_M = \Pi_j Exp(igX_j)$

Interaction graph obtained from quadratic objective function (MAXCUT)

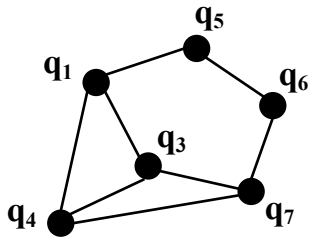


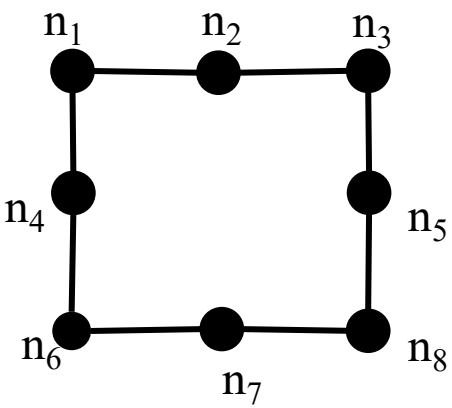
PS1	*MX*	*PS2*
P-S(q_1, q_4)	MIX(q_1)	P-S(q_1, q_4)
P-S(q_1, q_3)	MIX(q_3)	P-S(q_1, q_3)
P-S(q_3, q_4)	MIX(q_4)	P-S(q_3, q_4)
P-S(q_3, q_7)	MIX(q_5)	P-S(q_3, q_7)
P-S(q_4, q_7)	MIX(q_6)	P-S(q_4, q_7)
P-S(q_6, q_7)	MIX(q_7)	P-S(q_6, q_7)
P-S(q_5, q_6)		P-S(q_5, q_6)
P-S(q_1, q_5)		P-S(q_1, q_5)

- Every edge is a gate that needs to be executed (in arbitrary order)
- The same graph has to be executed multiple times (*p rounds*).
- Every qubit has to complete all the gates of round *p* before being involved in *p+1*

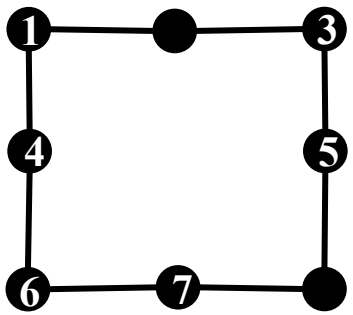
Circuit Execution Schedule

Interaction graph obtained from quadratic objective function (MAXCUT)



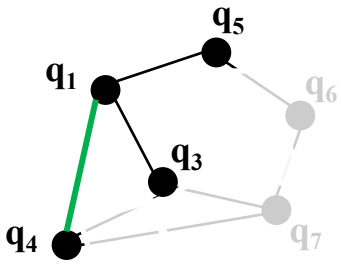


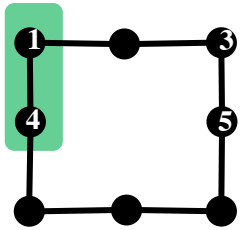
Initial assignment
$\mathbf{q_i \rightarrow n_i}$



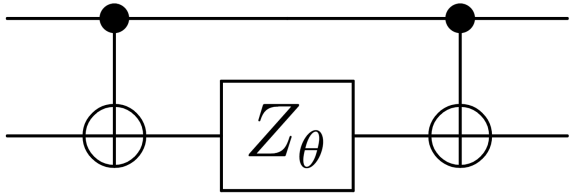
- Every edge is a gate that needs to be executed (in arbitrary order)
- The same graph has to be executed multiple times (*p rounds*).
- Every qubit has to complete all the gates of round *p* before being involved in *p+1*

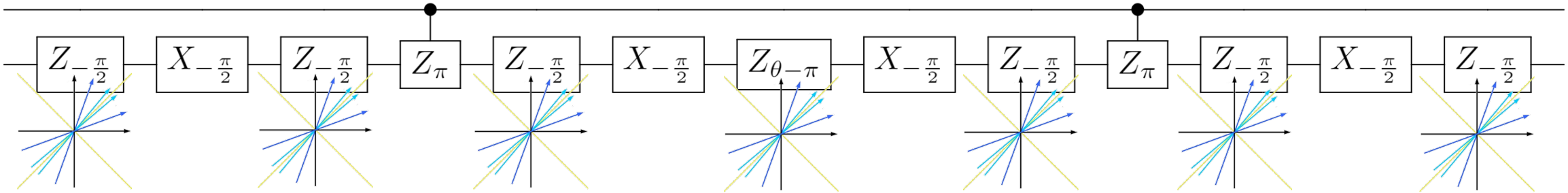
Circuit Execution Schedule

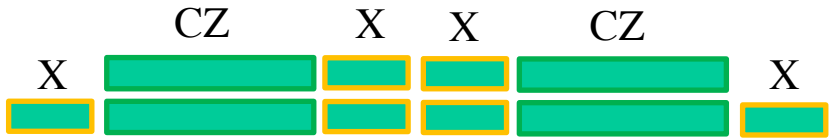




$\mathrm{Exp}(i\theta Z_1 Z_4)$ ZZ-Evolution Gate

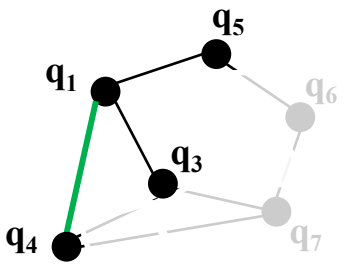


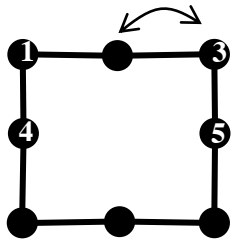




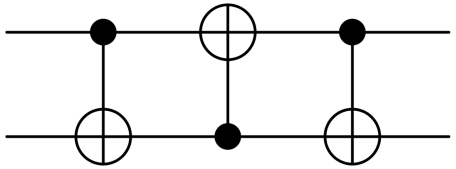
Duration $2\tau_2+4\tau_1$

Circuit Execution Schedule

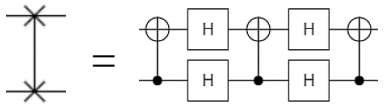


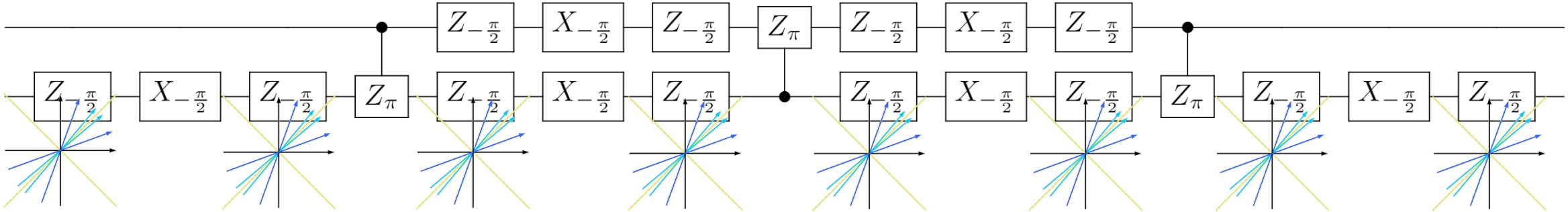


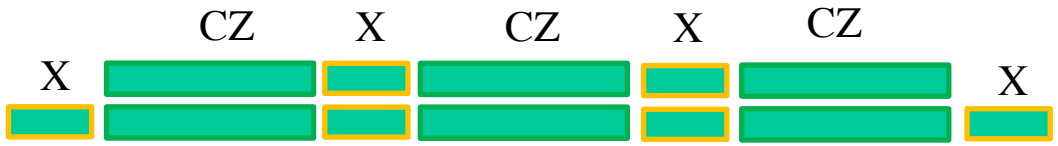
SWAP $|\Psi\rangle_3 \leftrightarrow |0\rangle$



From Unidirectional CNOTs to SWAP





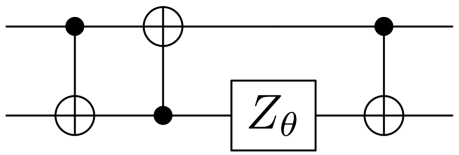


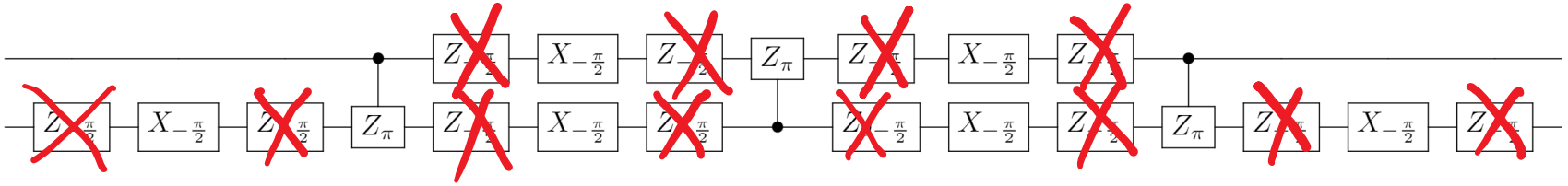
Duration $3\tau_2+4\tau_1$

Circuit Execution Schedule

SWAPS can also be inserted as part of the UZZ interaction without the need to be sequential.

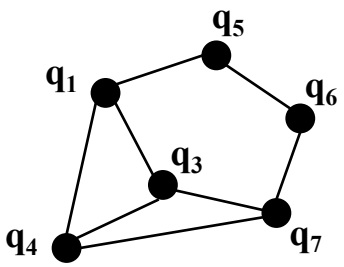
SWAP+ZZ-Evolution Gate

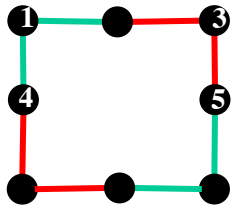




Duration $3\tau_2+4\tau_1$ (same as SWAP)

Circuit Execution Schedule

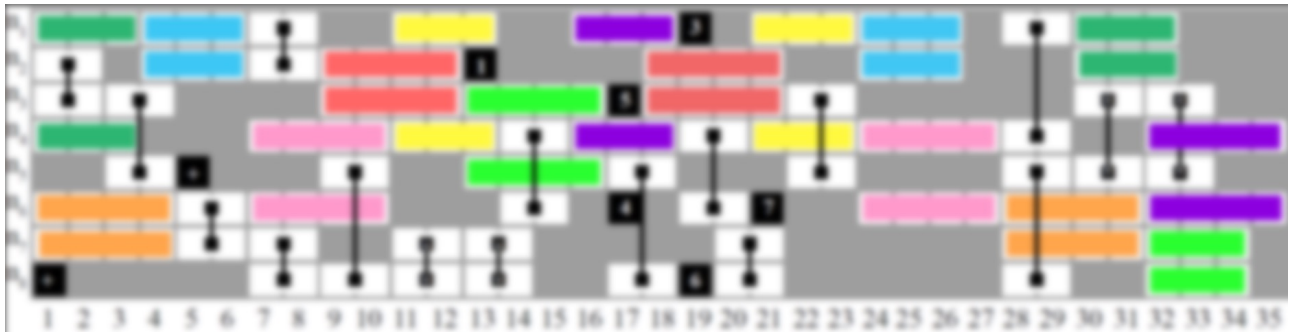




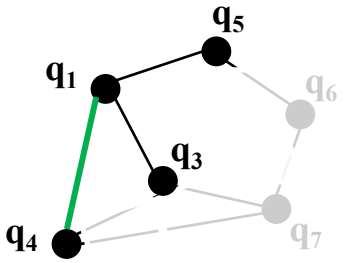
fast P-S (τ=3)
slow P-S (τ=4)
Swap (τ=2)

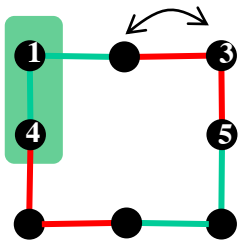
Benchmark presented at ICAPS17

Objective: finding the makespan-minimizing Gantt Schedule for p=1, p=2, N=8, N=21

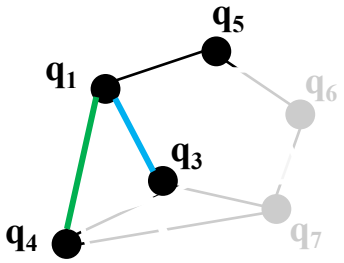


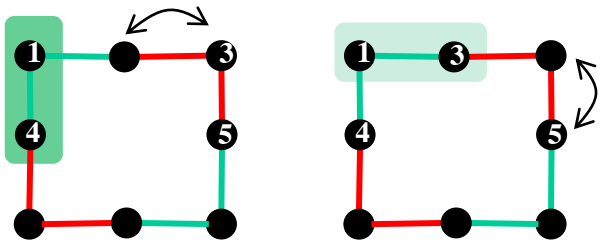
Circuit Execution Schedule



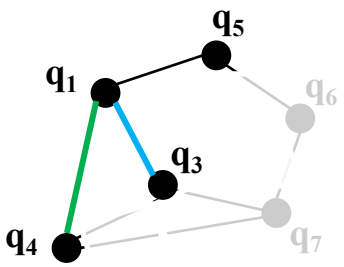


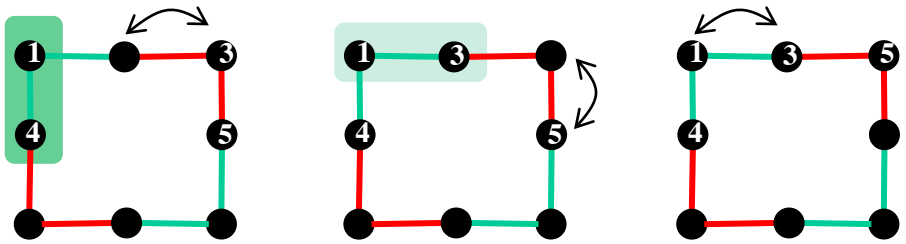
Circuit Execution Schedule



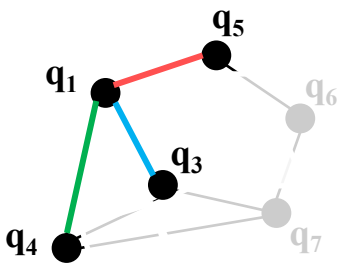


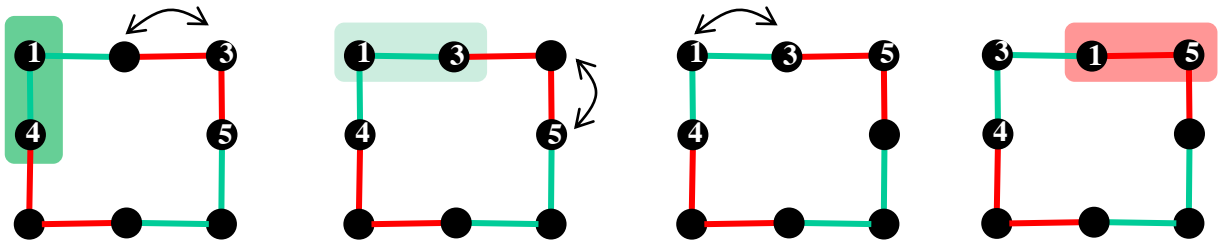
Circuit Execution Schedule

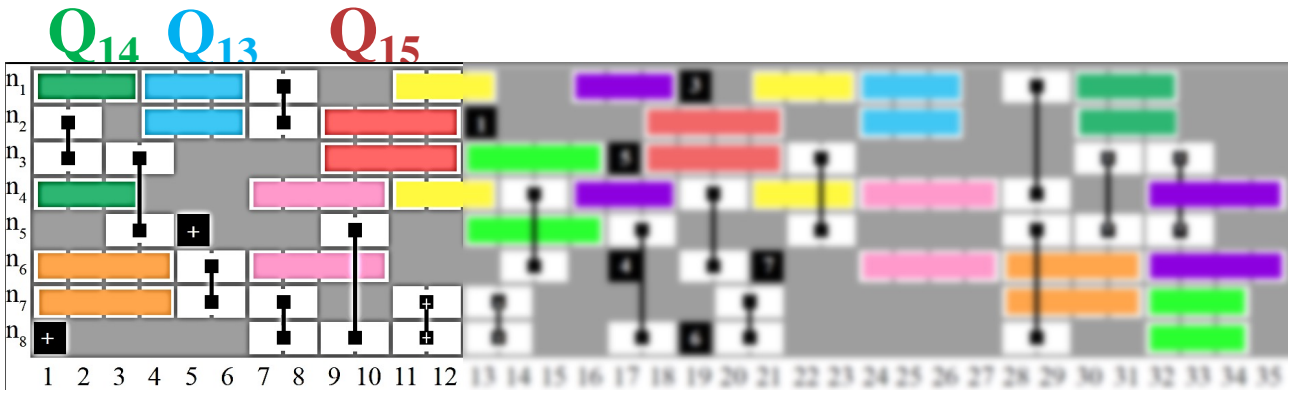




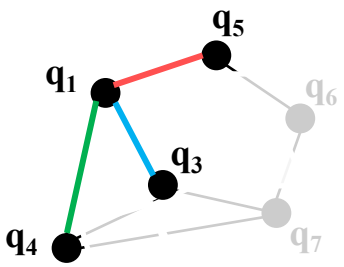
Circuit Execution Schedule

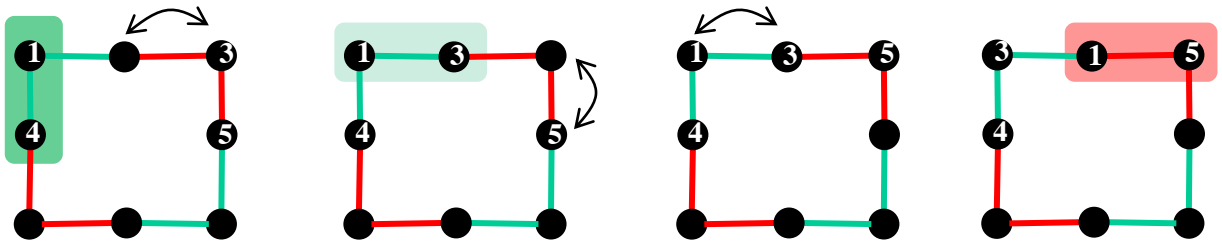




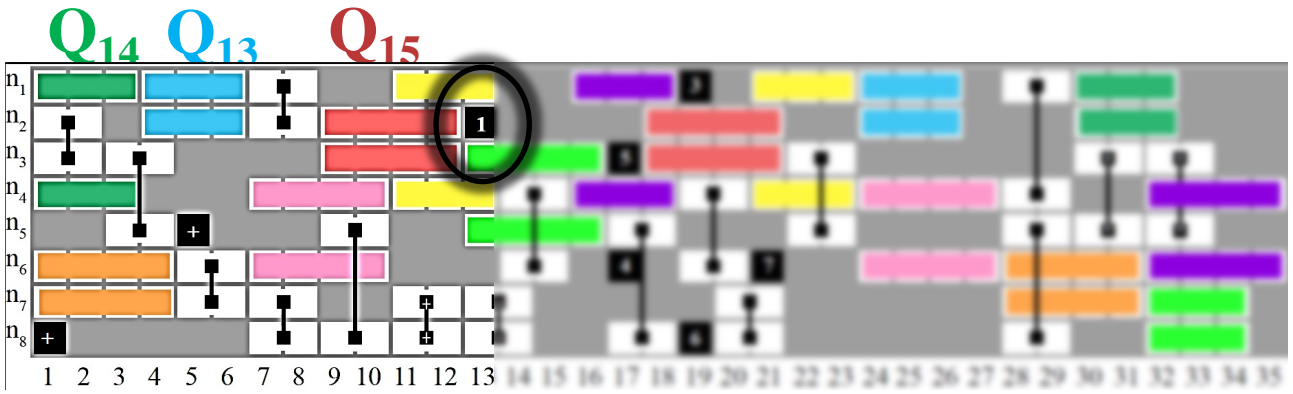


Circuit Execution Schedule

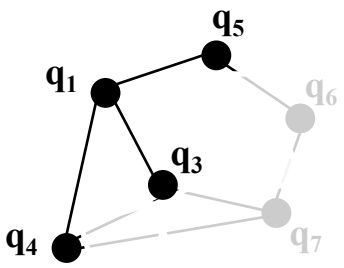


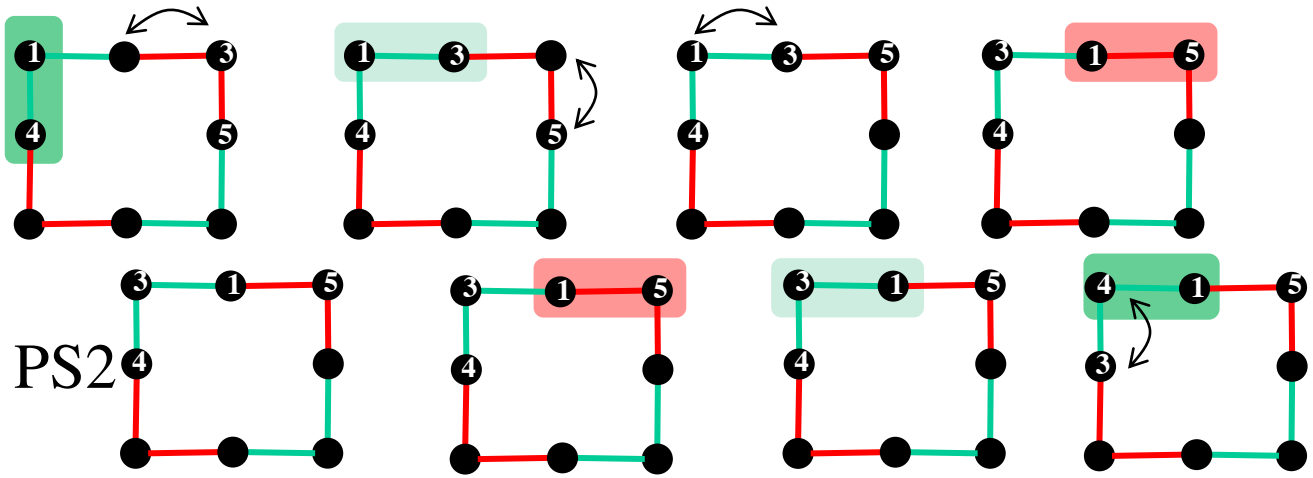


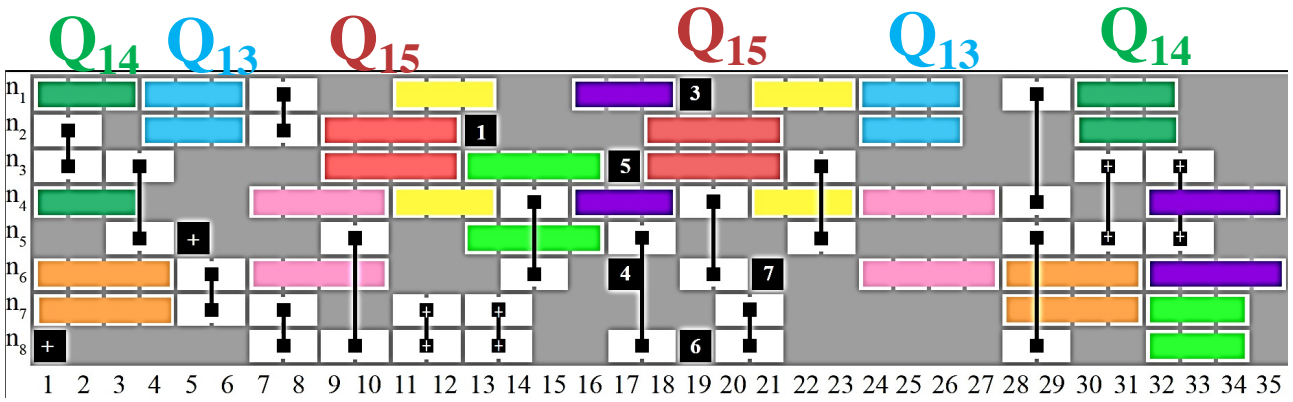
All actions of round 1 are completed – qubit can be mixed.
Qubit 1 can start participating to round 2.



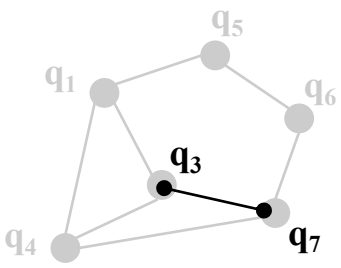
Circuit Execution Schedule

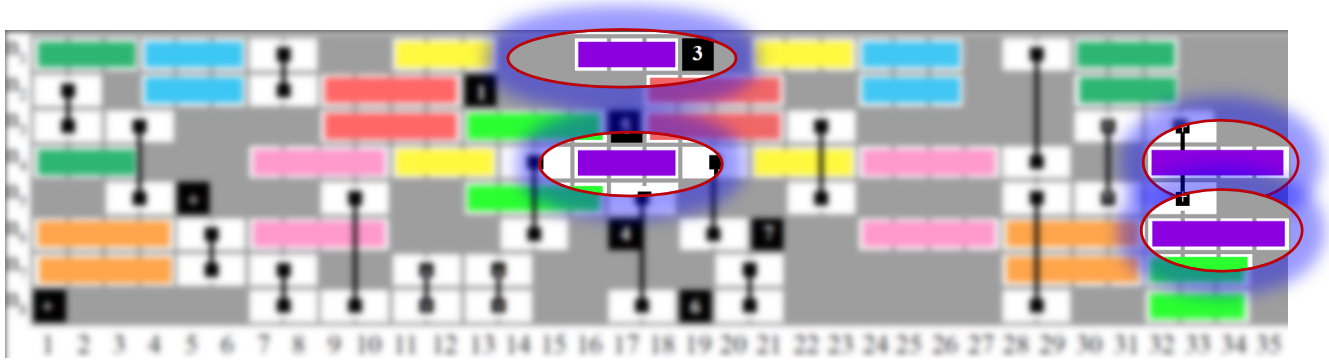




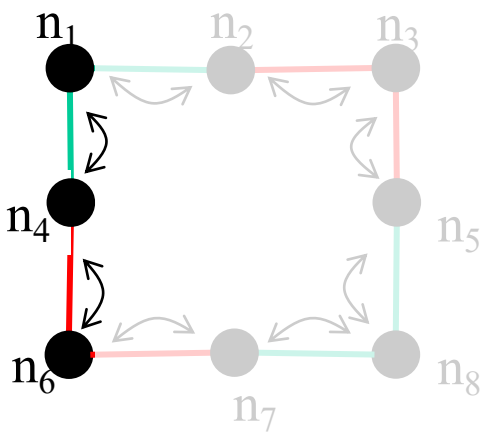


Circuit Execution Schedule





P-S(3,7) is fast on n_1, n_4
P-S(3,7) is slow on n_4, n_6



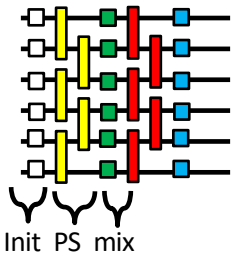
How to obtain these schedules efficiently?

Classical planning software is useful, and this is an active research field.

Why Hardware Efficiency

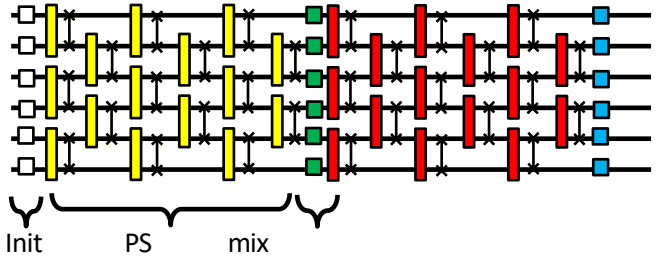
Hardware Efficiency is important for NISQ devices because:

- **It increases quantumness, leading to possibly supreme performance**
- **Faster circuit execution impact overall performance (speed/quality tradeoff)**

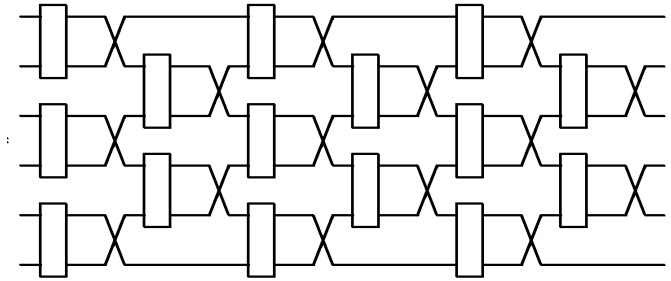


MaxCut QAOA on native graph (no swaps required, no XY gates)

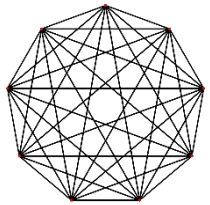
Sanity checks, detection of correlation between performance and fidelity or other improvements



MaxCut QAOA on fully connected graphs (**swaps** required, XY for compilation)



Swap network depth N with N(N-1)/2 gates



See Kivlichan Phys.Rev.Lett 120, 110501 (2018) and O'Gorman et al. ArXiv:1905.05118 (2019)

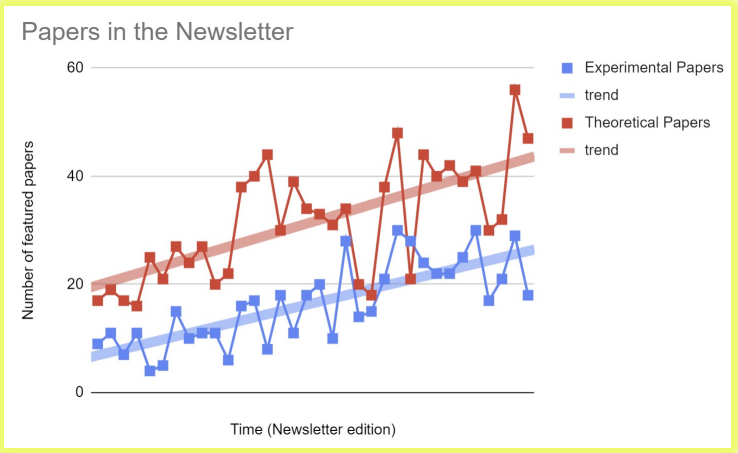
Problem: SWAPS are crazy expensive in the NISQ Era

Resources: NISQ Computing ArXiv Digest & SQMS ArXiv Digest

Monthly Newsletter on NISQ Applied Quantum Computing
https://riacs.usra.edu/quantum/nisqc-nl

- 1000+ subscribers
- ArXiv Digest ~70 papers a month
- Interfaced with http://metriq.info

- **NISQ Experiments**
  - Analog / Quantum Annealing
  - Atom Based
  - Photonic
  - Superconducting
  - Other
- **NISQ Algorithms**
  - Benchmarking; Software Tools; Compilation
  - Machine Learning
  - Optimization
  - Simulation
  - Other



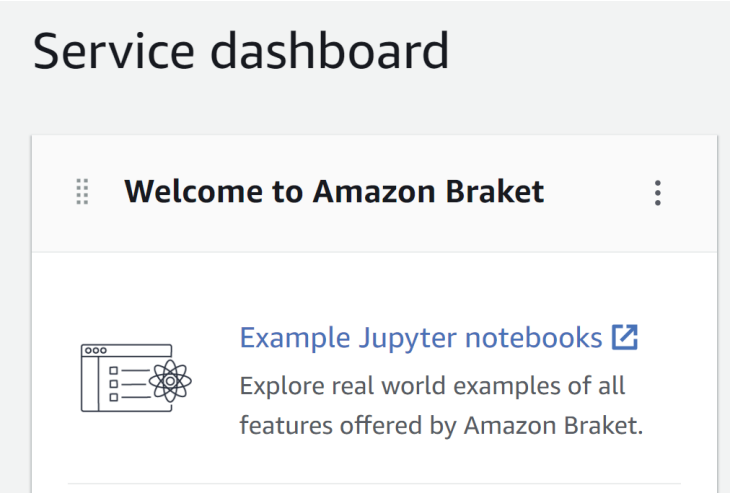
Amazon Braket for QAOA

https://github.com/aws/amazon-braket-examples/tree/main/examples/hybrid_quantum_algorithms/QAOA

main | amazon-braket-examples / examples / hybrid_quantum_algorithms / QAOA / | Go to file

shpface update examples to use Aspen M-2 device (#180) ... 8849796 on Aug 12 History

..		
QAOA_braket.ipynb	update examples to use Aspen M-2 device (#180)	2 months ago
hybrid_quantum.png	Folder structure changes, add notebook tests, format files	2 years ago
utils_classical.py	Fix some spelling (#101)	10 months ago
utils_qaoa.py	feat: remove s3 folder configuration and upgrade aspen references to ...	8 months ago



https://qbraid.com/haqs/