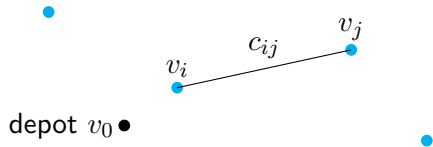


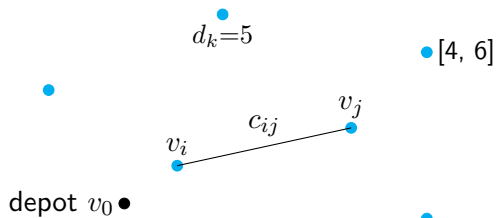
Seminar: Advanced Topics in Quantum Computing

On efficient encodings for QAOA
solutions to vehicle routing problems

Eben Jowie Haezer

December 1, 2023







<https://www.freepik.com/free-photos-vectors/airport-night/4>

<https://pictures.reuters.com/>

Adiabatic computation

A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum. [1]

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Adiabatic approximation

$$e^{A+B} = \lim_{n \rightarrow \infty} \left(e^{\frac{A}{n}} \cdot e^{\frac{B}{n}} \right)^n$$

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$$\forall A, B \in \mathbb{C}^{m \times m}. e^{A+B} = \lim_{n \rightarrow \infty} \left(e^{\frac{A}{n}} \cdot e^{\frac{B}{n}} \right)^n$$

$$\left([A, B] = 0 \implies e^{A+B} = e^A e^B \right)$$

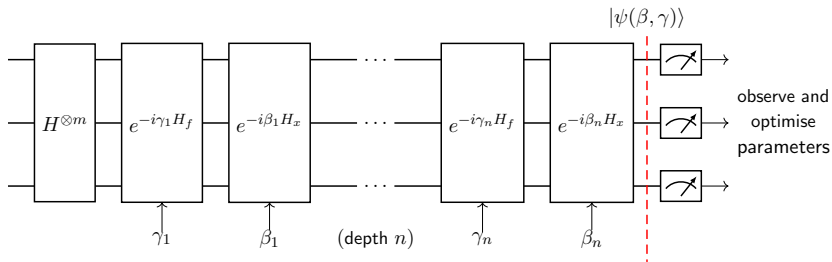
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[3]

QUBO

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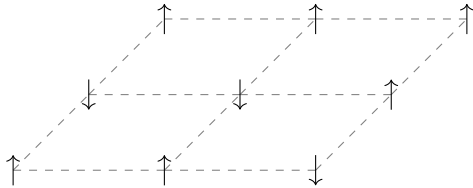
where $Q \in \mathbb{R}^{n \times n}$.

$$f_Q(x) = \langle x|Q|x\rangle = \sum_{i=1}^n \sum_{j=i}^n Q_{ij} x_i x_j$$

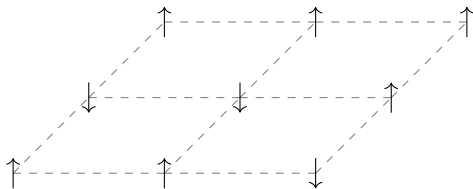
Problem	QUBO formulation
Number Partitioning (NP)	Glover et al. ¹
Maximum Cut (MC)	Glover et al. ¹
Minimum Vertex Cover (MVC)	Glover et al. ¹
Set Packing (SP)	Glover et al. ¹
Set Partitioning (SPP)	Glover et al. ¹
Maximum 2-SAT (M2SAT)	Glover et al. ¹
Maximum 3-SAT (M3SAT)	Dinneen et al. ²
Graph Coloring (GC)	Glover et al. ¹
General 0/1 Programming (G01P)	Glover et al. ¹
Quadratic Assignment (QA)	Glover et al. ¹
Quadratic Knapsack (QK)	Glover et al. ¹
Graph Partitioning	Lucas ³
Decisional Clique Problem	Lucas ³
Maximum Clique Problem	Chapuis ¹⁹
Binary Integer Linear Programming	Lucas ³
Exact Cover	Lucas ³
3SAT	Lucas ³
Maximal Independent Set	Djidjev et al. ⁴
Minimal Maximal Matching	Lucas ³
Set Cover	Lucas ³
Knapsack with Integer Weights	Lucas ³
Clique Cover	Lucas ³
Job Sequencing Problem	Lucas ³
Hamiltonian Cycles Problem	Lucas ³
Minimal Spanning Tree	Lucas ³
Steiner Trees	Lucas ³
Directed Feedback Vertex Set	Lucas ³
Undirected Feedback Vertex Set	Lucas ³
Feedback Edge Set	Lucas ³
Traveling Salesman (TSP)	Lucas ³
Traveling Salesman with Time Windows (TSPTW)	Papadimitras et al. ¹ , Salehi et al. ⁵
Graph Isomorphism	Calude et al. ⁶
Subgraph Isomorphism	Calude et al. ⁶
Induced Subgraph	Calude et al. ⁶
Capacitated Vehicle Routing (CVRP)	Irie et al. ⁷ , Feld et al. ¹⁰
Multi-Depot Capacitated Vehicle Routing (MDCVRP)	Harikrishnakumar et al. ⁸
1-n Norm	Yehoda et al. ⁹
k-Models	Bouschagel et al. ¹⁸
Contact Map Overlap Problem	Oliveira et al. ¹¹
Minimum Multicut Problem	Cruz-Santos et al. ¹²
Broadcast Time Problem	Calude et al. ¹³
Maximum Common Subgraph Isomorphism	Huang et al. ¹⁴
Densest k-subgraph	Calude et al. ¹⁵
Longest Path Problem	McCollum et al. ¹⁶
Airport Gateway Assignment	Stollenwerk et al. ¹⁸
Linear regression	Date et al. ¹⁷
Support Vector Machine	Date et al. ¹⁷
k-means clustering	Date et al. ¹⁷
Eigentrality	Prosser et al. ¹⁸
Container Assignment Problem	Phillipson et al. ²⁰
k-colorable subgraph problem	Rodolfo et al. ²²
Routing and Wavelength Assignment with Protection	Oylum et al. ²¹
Aircraft Loading Optimization	Giovanni et al. ²⁴
Linear least squares / system of linear equations	Ajinkya et al. ²⁵
Traffic Flow Optimization	Neukart et al. ²⁶
Permutation Synchronization	Tolga et al. ²⁷
Max-Flow Problem	Krauss et al. ²⁸
Network Shortest Path Problem	Krauss et al. ²⁹
Structural Isomer Search Problem	Terry et al. ¹⁸

k-densest Common Sub-Graph Isomorphism	Huang et al. ³⁰
Community Detection	Negre et al. ³¹
Nurse Scheduling problem	Ikeeda et al. ³⁴
Aircraft Loading Optimization	Pilon et al. ³⁵
PageRank	Garrone et al. ³⁶
Ramsey numbers	Gaitan et al. ³⁷
Generalized Ramsey numbers	Ranjbar et al. ³⁸
Transaction Settlement	Braine et al. ³⁹
Sensor placement problem in water distribution networks	Spezialti et al. ⁴⁰
Fault Detection and Diagnosis of Graph-Based Systems	Perdomo-Ortiz et al. ⁴¹
Bounded-Depth Steiner Trees	Liu et al. ⁴²
Graph Matching with Permutation Matrix Constraints	Benkner et al. ⁴³
Gaussian Process Variance Reduction	Bottarelli et al. ⁴⁴
Quantum Permutation Synchronization	Birdal et al. ⁴⁵
Unit Commitment Problem	Ajagekar et al. ⁴⁶
Heat Exchanger Network Synthesis	Ajagekar et al. ⁴⁶
Garden Optimization Problem	Caluca et al. ⁴⁷
Two-Dimensional Cutting Stock Problem	Arai et al. ⁴⁸
Labelled Maximum Weighted Common Subgraph	Hernandez et al. ⁴⁹
Maximum Weighted Co-k-plex	Hernandez et al. ⁴⁹
Molecular Similarity based on Graphs	Hernandez et al. ⁴⁹ (*)
Portfolio Optimization (Modern Portfolio Theory)	Palmer et al. ⁵⁰ , Phillipson et al. ⁵¹
Weighted Maximum Cut	Pelofske et al. ⁵³
Weighted Maximum Clique	Pelofske et al. ⁵³
Satellite Scheduling	Stollenwerk et al. ⁵⁴
Refinery Scheduling	Ossorio-Cuicillo et al. ⁵⁵
Job Shop Scheduling	Venturelli et al. ⁵⁶
Extended Job Shop Scheduling with Autonomous Ground Vehicles	Geitz et al. ⁷⁰
Parallel Flexible Job Shop Scheduling	Denkova et al. ⁵⁷
Bin Packing with Integer Weights	Lodewijks ⁵⁸ (Alternative: ref ⁵⁹)
Minimum Partitioning with m sets	Lodewijks ⁵⁸
Graph Partitioning with k sets	Lodewijks ⁵⁸
Subset Sum Problem	Lodewijks ⁵⁸
Numerical Three-Dimensional Matching	Lodewijks ⁵⁸
Social Workers Problem	Adelmann et al. ⁵⁹
EV-Bus Charging Scheduling Problem	Yu et al. ⁶¹
Vehicle Routing Problem	Borowski et al. ⁶⁰
Robot Path Planning	Fitzgner et al. ⁶²
Scheduling on Undirected Hamiltonian Paths	Rieffel et al. ⁶³
Market Graph Clustering	Hong et al. ⁶⁴
Balanced k-Means Clustering	Arthur et al. ⁶⁵
Distance-based Clustering in general	Matsumoto et al. ⁶⁶
Credit Scoring and Classification	Malne et al. ⁶⁸
Dynamic Portfolio Optimization	Mugel et al. ⁶⁸
Railway Dispatching and Conflict Management	Domino et al. ⁷⁰
Optimization	Domino et al. ⁷⁰
Workflow Application Scheduling	Tomasiewicz et al. ⁷¹
Mixed Round-Robin Tournament	Karamata et al. ⁷²
Transaction Scheduling	Blittner et al. ⁷⁴
Transformation Estimation	Golyanik et al. ⁷⁵
Point Set Registration	Golyanik et al. ⁷⁵
Maximum Cardinality Matching	Vert et al. ⁷⁶
Multi-car Paint Shop Optimization	Tarkoni et al. ⁷⁷
Binary Paint Shop Problem	Streif et al. ⁷⁸

Ising model

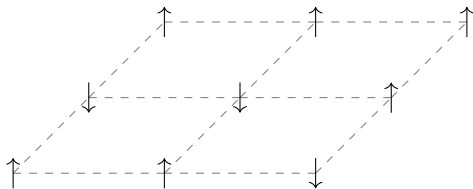


Ising model



$$H = - \sum_{\langle i j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \mu \sum_i h_i^z \sigma_i^z - \mu \sum_i h_i^x \sigma_i^x$$

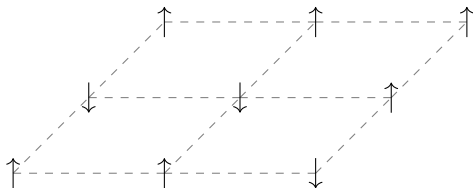
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$$\sigma \mapsto 2x - 1, \quad x \in \{0,1\}$$

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$$\Delta = \sum_{b=0}^{\lceil \log_2 1+m \rceil - 1} 2^b a_b^r, \quad a_b^r \in \{0, 1\}$$

Two phase procedure

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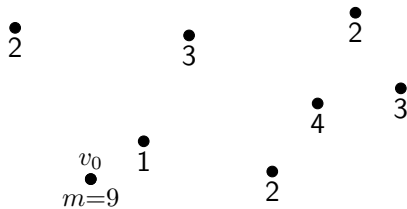
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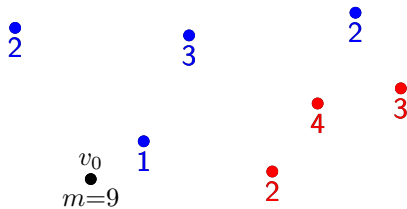
divide and conquer [8] [9]

- clustering phase
- routing phase

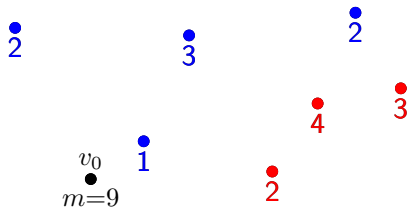
Clustering



Clustering

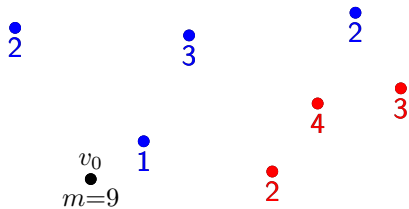


Clustering



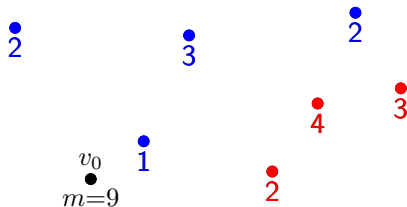
subject to constraints:

Clustering



subject to constraints: **once**, **cap**

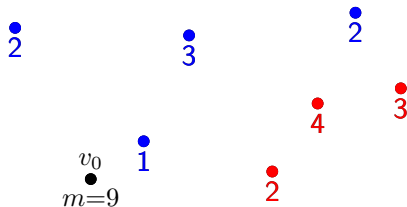
Clustering



subject to constraints: **once**, **cap**

additional constraint: **cluster**

Clustering

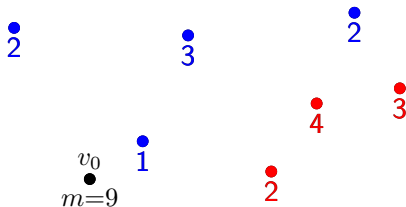


subject to constraints: **once**, **cap**

additional constraint: **cluster**

The cumulative edge cost c_{ij} between all pairs of nodes (i, j) within a cluster should be minimal.

Clustering



subject to constraints: **once, cap**

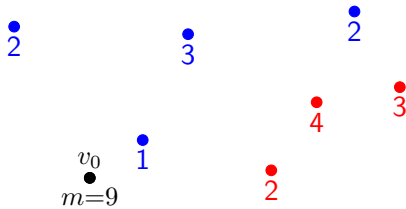
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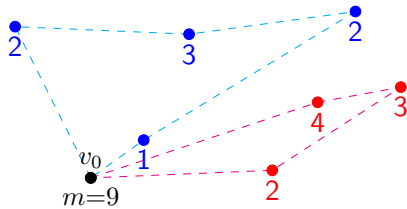
$$H_{\text{cluster}} = \sum_r \sum_{i, j} c_{ij} x_i^r x_j^r$$

$$\text{where } x_i^r = \sum_t x_{i,t}^k$$

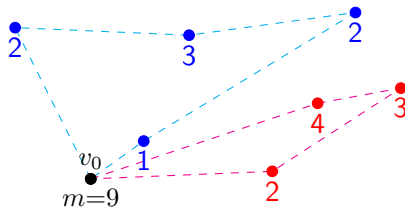
Routing



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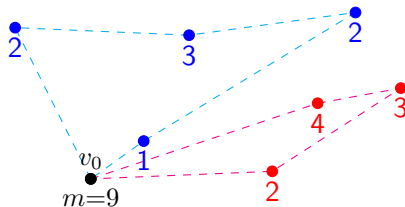


Routing



subject to constraints: **once**, **step**, edge costs

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$$H_{\text{tsp}} = q_1 H_{\text{once}} + q_2 H_{\text{step}} + q_3 H_c$$

Complete encoding

$$\left. \begin{array}{ccc} \text{---} & \dots & \text{---} \\ \text{---} & \dots & \text{---} \\ \text{---} & \dots & \text{---} \end{array} \right\} |\psi\rangle$$

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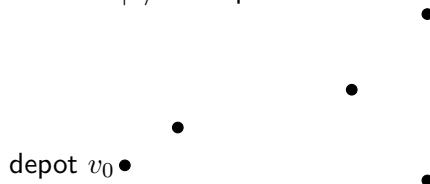
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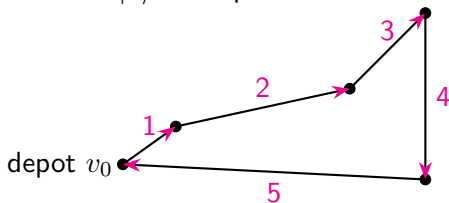


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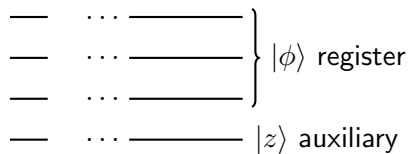
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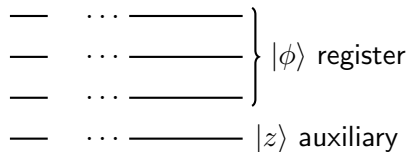


Minimal encoding

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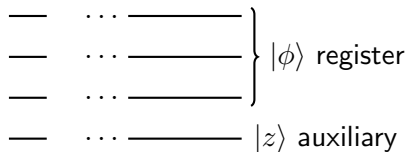


Minimal encoding



register width n_r , aux width n_a , $n_q = n_r + n_a$

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$$|\psi(\theta)\rangle = \sum_{i=1}^{n_c} \beta_k(a_i|0\rangle + b_i|1\rangle) |\phi_i\rangle$$

Minimal encoding

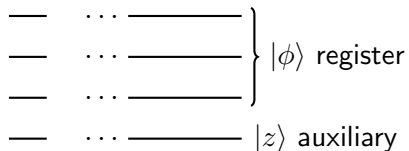
$$\begin{array}{c} \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \end{array} \left. \vphantom{\begin{array}{c} \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \end{array}} \right\} |\phi\rangle \text{ register}$$
$$\text{---} \quad \dots \text{---} \quad |z\rangle \text{ auxiliary}$$

register width n_r , aux width n_a , $n_q = n_r + n_a$

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$$n_q = 1 + \log_2 n_c$$

Example

let $n_c = 4$, $n_r = 2$.

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Tradeoffs

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$$\begin{aligned} \text{cov}(x_i, x_j) &= \mathbb{E} x_i x_j - \mathbb{E} x_i \mathbb{E} x_j \\ &= 0 \end{aligned}$$

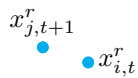
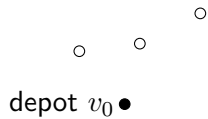
Tradeoffs



Tradeoffs



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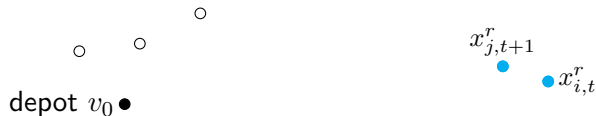


Tradeoffs



$$|\psi(\theta)\rangle = \sum_{i=1}^{n_c} \beta_k(a_i|0\rangle + b_i|1\rangle) |\phi_i\rangle$$

Tradeoffs

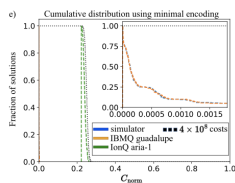
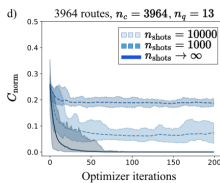
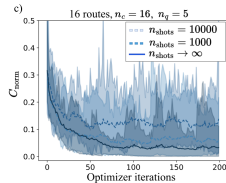
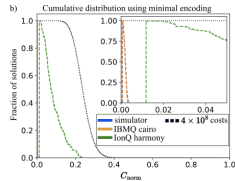
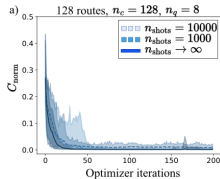
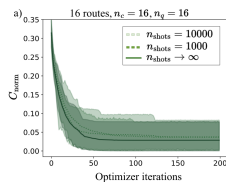


$$|\psi(\theta)\rangle = \sum_{i=1}^{n_c} \beta_k(a_i|0\rangle + b_i|1\rangle) |\phi_i\rangle$$

example:

$$|\psi^*\rangle = \frac{1}{2}(|1\rangle|00\rangle + |1\rangle|01\rangle + |1\rangle|10\rangle + |0\rangle|11\rangle)$$

Experimental results



[11]

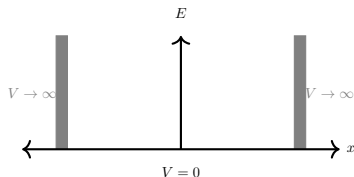
Thank you for your attention.

`github.com/ge42faz/qsem-23w`

Backup slides

Backup slides

Adiabatic computation

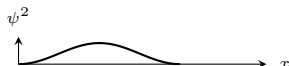
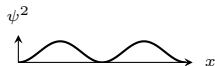


$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t)$$

$$\psi(x, t) = e^{-i\omega t} (A \sin kx + B \cos kx) \text{ for } x \text{ within the box.}$$

Backup slides

Adiabatic computation



$$H|\psi\rangle = E|\psi\rangle$$

$$E_k = \hbar\omega_k = \frac{n^2\pi^2}{L^2} \frac{\hbar^2}{2m}$$

$$H(t) = \left(1 - \frac{t}{T}\right) \cdot H_0 + \frac{t}{T} \cdot H_p$$

$$0 \leq t \leq 1, T \in \mathcal{O}\left(\frac{1}{g^2}\right)$$

$$[H_0, H_p] \neq 0$$

Backup slides

Ising model

$$\mathbf{B} = \frac{\mu_0}{4\pi} \left(\frac{3\mathbf{r}(\mathbf{m} \cdot \mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3} \right)$$

$$H = - \sum_{\langle i j \rangle} J_{ij} \sigma_i \sigma_j + \mu \sum_i h_i \sigma_i$$

$$\mu = \frac{-e}{2m_e} L$$

$J_{ij} > 0$ ferromagnetic, $J_{ij} < 0$ antiferromagnetic.

$$C_{\text{cpl}}(\theta) = \langle H \rangle = \langle \psi(\theta) | H | \psi(\theta) \rangle$$

$$\begin{aligned} C_{\text{min}}(\theta) &= \sum_{i \neq j}^{n_c} Q_{ij} \|b_i\|^2 \|b_j\|^2 + \sum_{i=1}^{n_c} Q_{ii} \|b_i\|^2 \\ &= \sum_{i \neq j}^{n_c} Q_{ij} \frac{\langle P_i^1 \rangle}{\langle P_i \rangle} \frac{\langle P_j^1 \rangle}{\langle P_j \rangle} + \sum_{i=1}^{n_c} Q_{ii} \frac{\langle P_i^1 \rangle}{P_i} \end{aligned}$$

expressed as projectors $P_i = |\phi_i\rangle\langle\phi_i|$ and $P_i^1 = |1\rangle\langle 1| \otimes P_i$.

$$\overline{C} = \frac{C(\theta) - C^*}{\Delta C}$$

Backup slides

QAOA

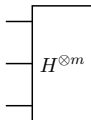
$$|\psi(\beta, \gamma)\rangle =$$

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QAOA

$$|\psi(\beta, \gamma)\rangle =$$

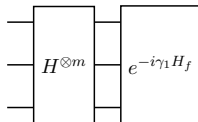
$$|+\rangle^{\otimes m}$$



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QAOA

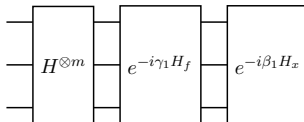
$$|\psi(\beta, \gamma)\rangle = e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$



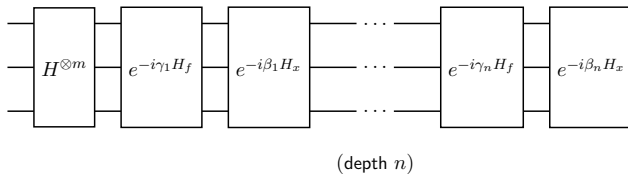
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QAOA

$$|\psi(\beta, \gamma)\rangle = e^{-i\beta_k H_x} e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$



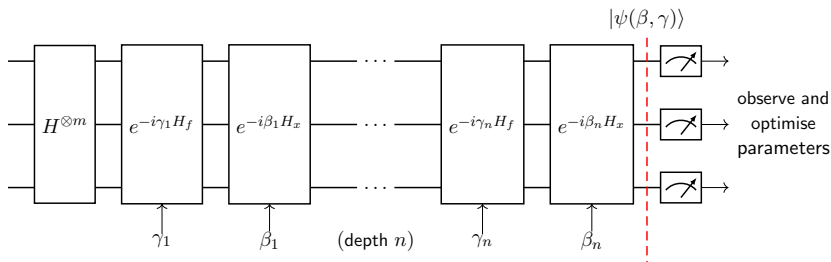
$$|\psi(\beta, \gamma)\rangle = \prod_k e^{-i\beta_k H_x} e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$








Backup slides





QAOA

$$|\psi(\beta, \gamma)\rangle = \prod_k e^{-i\beta_k H_x} e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$





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