

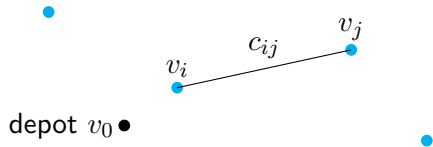
# Seminar: Advanced Topics in Quantum Computing

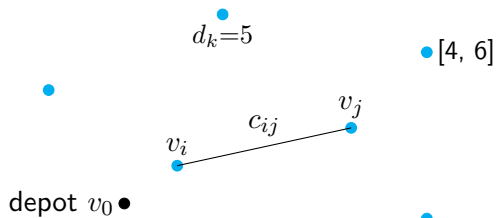
On efficient encodings for QAOA  
solutions to vehicle routing problems

Eben Jowie Haezer

December 2, 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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$$H(t) = \left(1 - \frac{t}{T}\right) \cdot H_0 + \frac{t}{T} \cdot H_p$$

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



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

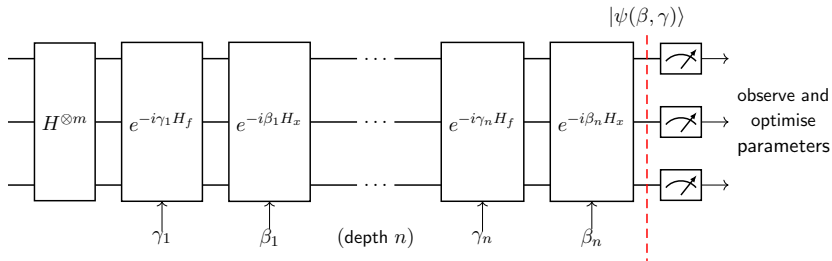
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$$|\psi(\beta, \gamma)\rangle = \prod_k e^{-i\beta_k H_x} e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$

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[3]

QUBO

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

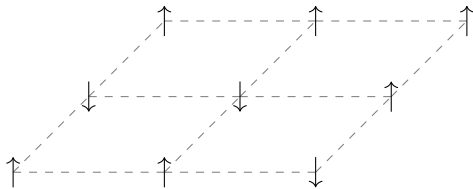
$$f_Q(x) = \langle x|Q|x\rangle = \sum_{i=1}^n \sum_{j=i}^n Q_{ij} x_i x_j$$

Problem	QUBO formulation
Number Partitioning (NP)	Glover et al. <sup>1</sup>
Maximum Cut (MC)	Glover et al. <sup>2</sup>
Minimum Vertex Cover (MVC)	Glover et al. <sup>2</sup>
Set Packing (SP)	Glover et al. <sup>2</sup>
Set Partitioning (SPP)	Glover et al. <sup>2</sup>
Maximum 2-SAT (M2SAT)	Glover et al. <sup>2</sup>
Maximum 3-SAT (M3SAT)	Dinneen et al. <sup>3</sup>
Graph Coloring (GC)	Glover et al. <sup>2</sup>
General 0/1 Programming (G01P)	Glover et al. <sup>2</sup>
Quadratic Assignment (QA)	Glover et al. <sup>2</sup>
Quadratic Knapsack (QK)	Glover et al. <sup>2</sup>
Graph Partitioning	Lucas <sup>4</sup>
Decisional Clique Problem	Lucas <sup>4</sup>
Maximum Clique Problem	Chapuis <sup>5</sup>
Binary Integer Linear Programming	Lucas <sup>4</sup>
Exact Cover	Lucas <sup>4</sup>
3SAT	Lucas <sup>4</sup>
Maximal Independent Set	Djidjev et al. <sup>6</sup>
Minimal Maximal Matching	Lucas <sup>4</sup>
Set Cover	Lucas <sup>4</sup>
Knapsack with Integer Weights	Lucas <sup>4</sup>
Clique Cover	Lucas <sup>4</sup>
Job Sequencing Problem	Lucas <sup>4</sup>
Hamiltonian Cycles Problem	Lucas <sup>4</sup>
Minimal Spanning Tree	Lucas <sup>4</sup>
Steiner Trees	Lucas <sup>4</sup>
Directed Feedback Vertex Set	Lucas <sup>4</sup>
Undirected Feedback Vertex Set	Lucas <sup>4</sup>
Feedback Edge Set	Lucas <sup>4</sup>
Traveling Salesman (TSP)	Lucas <sup>4</sup>
Traveling Salesman with Time Windows (TSPTW)	Papadimitras et al. <sup>1</sup> , Salehi et al. <sup>7</sup>
Graph Isomorphism	Calude et al. <sup>8</sup>
Subgraph Isomorphism	Calude et al. <sup>8</sup>
Induced Subgraph	Calude et al. <sup>8</sup>
Capacitated Vehicle Routing (CVRP)	Irie et al. <sup>9</sup> , Feld et al. <sup>10</sup>
Multi-Depot Capacitated Vehicle Routing (MDCVRP)	Harikrishnakumar et al. <sup>6</sup>
1-n Norm	Yehoda et al. <sup>11</sup>
k-Models	Bouschagel et al. <sup>12</sup>
Contact Map Overlap Problem	Oliveira et al. <sup>13</sup>
Minimum Multicut Problem	Cruz-Santos et al. <sup>12</sup>
Broadcast Time Problem	Calude et al. <sup>13</sup>
Maximum Common Subgraph Isomorphism	Huang et al. <sup>14</sup>
Densest k-subgraph	Calude et al. <sup>15</sup>
Longest Path Problem	McCullum et al. <sup>16</sup>
Airport Gateway Assignment	Stollenwerk et al. <sup>18</sup>
Linear regression	Date et al. <sup>17</sup>
Support Vector Machine	Date et al. <sup>17</sup>
k-means clustering	Date et al. <sup>17</sup>
Eigentraility	Prosser et al. <sup>18</sup>
Container Assignment Problem	Phillipson et al. <sup>19</sup>
k-colorable subgraph problem	Rodolfo et al. <sup>22</sup>
Routing and Wavelength Assignment with Protection	Oylum et al. <sup>23</sup>
Aircraft Loading Optimization	Giovanni et al. <sup>24</sup>
Linear least squares / system of linear equations	Ajinkya et al. <sup>25</sup>
Traffic Flow Optimization	Neukart et al. <sup>26</sup>
Permutation Synchronization	Tolga et al. <sup>27</sup>
Max-Flow Problem	Krauss et al. <sup>28</sup>
Network Shortest Path Problem	Krauss et al. <sup>29</sup>
Structural Isomer Search Problem	Terry et al. <sup>30</sup>

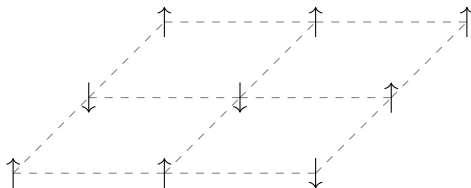
k-densest Common Sub-Graph Isomorphism	Huang et al. <sup>32</sup>
Community Detection	Negre et al. <sup>33</sup>
Nurse Scheduling problem	Ikeeda et al. <sup>34</sup>
Aircraft Loading Optimization	Pilon et al. <sup>35</sup>
PageRank	Garrone et al. <sup>36</sup>
Ramsey numbers	Gaitan et al. <sup>37</sup>
Generalized Ramsey numbers	Ranjbar et al. <sup>38</sup>
Transaction Settlement	Braine et al. <sup>39</sup>
Sensor placement problem in water distribution networks	Spezialini et al. <sup>40</sup>
Fault Detection and Diagnosis of Graph-Based Systems	Perdomo-Ortiz et al. <sup>41</sup>
Bounded-Depth Steiner Trees	Liu et al. <sup>42</sup>
Graph Matching with Permutation Matrix Constraints	Benkhar et al. <sup>43</sup>
Gaussian Process Variance Reduction	Bottarelli et al. <sup>44</sup>
Quantum Permutation Synchronization	Birdal et al. <sup>45</sup>
Unit Commitment Problem	Ajagekar et al. <sup>46</sup>
Heat Exchanger Network Synthesis	Ajagekar et al. <sup>46</sup>
Garden Optimization Problem	Caluca et al. <sup>47</sup>
Two-Dimensional Cutting Stock Problem	Arai et al. <sup>48</sup>
Labelled Maximum Weighted Common Subgraph	Hernandez et al. <sup>49</sup>
Maximum Weighted Co-k-plex	Hernandez et al. <sup>49</sup>
Molecular Similarity based on Graphs	Hernandez et al. <sup>49</sup> (*)
Portfolio Optimization (Modern Portfolio Theory)	Palmer et al. <sup>50</sup> , Phillipson et al. <sup>51</sup>
Weighted Maximum Cut	Pelofske et al. <sup>53</sup>
Weighted Maximum Clique	Pelofske et al. <sup>53</sup>
Satellite Scheduling	Stollenwerk et al. <sup>54</sup>
Refinery Scheduling	Ossorio-Cuicillo et al. <sup>55</sup>
Job Shop Scheduling	Venturelli et al. <sup>56</sup>
Extended Job Shop Scheduling with Autonomous Ground Vehicles	Geitz et al. <sup>72</sup>
Parallel Flexible Job Shop Scheduling	Denkova et al. <sup>57</sup>
Bin Packing with Integer Weights	Lodewijks <sup>58</sup> (Alternative: ref)
Minimum Partitioning with m sets	Lodewijks <sup>58</sup>
Graph Partitioning with k sets	Lodewijks <sup>58</sup>
Subset Sum Problem	Lodewijks <sup>58</sup>
Numerical Three-Dimensional Matching	Lodewijks <sup>58</sup>
Social Workers Problem	Adelmann et al. <sup>59</sup>
EV-Bus Charging Scheduling Problem	Yu et al. <sup>61</sup>
Vehicle Routing Problem	Borowski et al. <sup>60</sup>
Robot Path Planning	Fitzgaur et al. <sup>62</sup>
Scheduling on Undirected Hamiltonian Paths	Rieffel et al. <sup>63</sup>
Market Graph Clustering	Hong et al. <sup>64</sup>
Balanced k-Means Clustering	Arthur et al. <sup>65</sup>
Distance-based Clustering in general	Matsumoto et al. <sup>66</sup>
Credit Scoring and Classification	Malne et al. <sup>68</sup>
Dynamic Portfolio Optimization	Mugel et al. <sup>68</sup>
Railway Dispatching and Conflict Management	Domino et al. <sup>70</sup>
Optimization	Domino et al. <sup>70</sup>
Workflow Application Scheduling	Tomasiewicz et al. <sup>71</sup>
Mirrored Double Round-robin Tournament	Karamata et al. <sup>72</sup>
Transaction Scheduling	Blittner et al. <sup>74</sup>
Transformation Estimation	Golyanik et al. <sup>75</sup>
Point Set Registration	Golyanik et al. <sup>75</sup>
Maximum Cardinality Matching	Vert et al. <sup>76</sup>
Multi-car Paint Shop Optimization	Tarkoni et al. <sup>77</sup>
Binary Paint Shop Problem	Streif et al. <sup>78</sup>



# Ising model

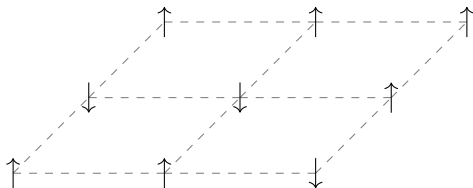


# Ising model



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

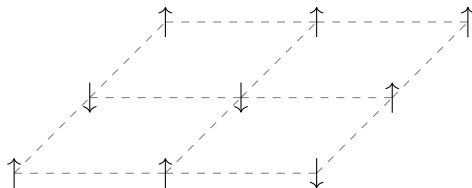
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$$\sigma \mapsto 2x - 1, \quad x \in \{0,1\}$$

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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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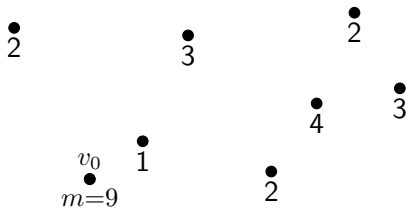
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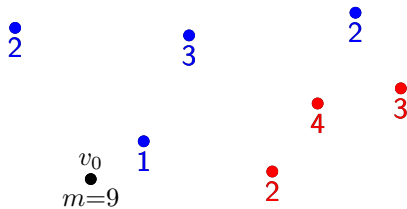
divide and conquer [8] [9]

- clustering phase
- routing phase

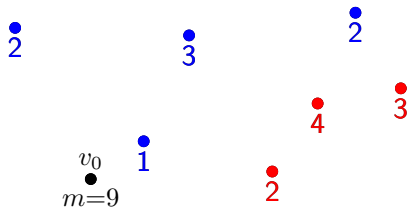
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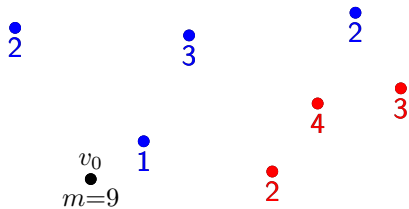
# Clustering



subject to constraints:

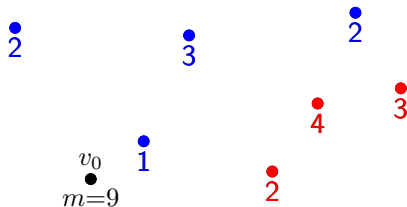


# Clustering



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

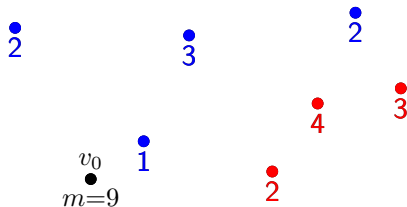
# Clustering



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

additional constraint: **cluster**

# Clustering

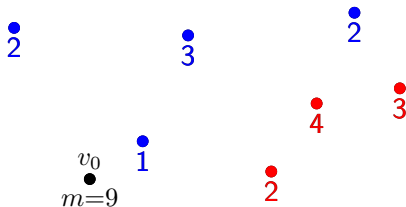


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*The cumulative edge cost  $c_{ij}$  between all pairs of nodes  $(i, j)$  within a cluster should be minimal.*

# Clustering



subject to constraints: **once, cap**

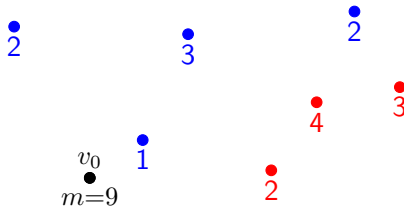
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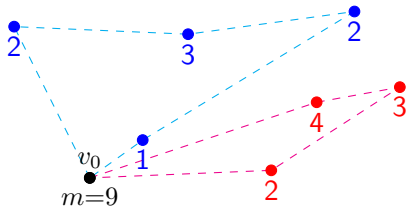
$$H_{\text{cluster}} = \sum_r \sum_{i, j} c_{ij} x_i^r x_j^r$$

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

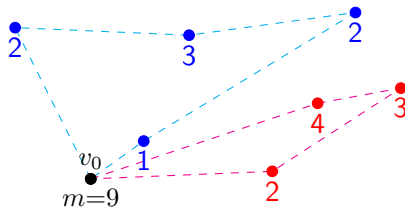
# Routing



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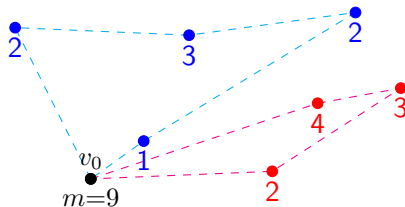


# Routing



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

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

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



# Complete encoding

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

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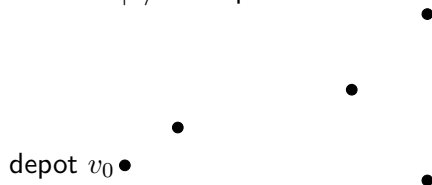
$$|\psi\rangle = \sum_{z \in \{0,1\}^n} \beta_z |z\rangle$$

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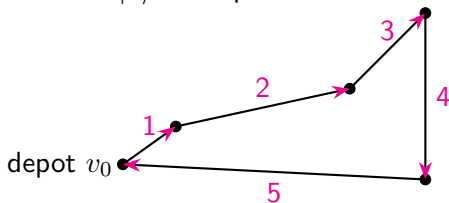


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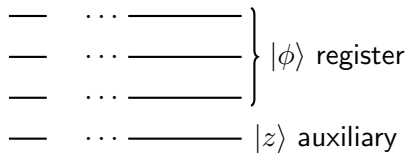
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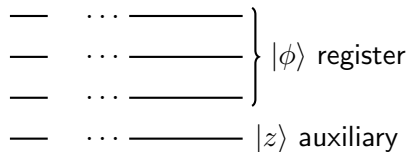


# Minimal encoding

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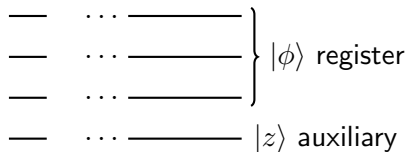


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register width  $n_r$ , aux width  $n_a$ ,  $n_q = n_r + n_a$

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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

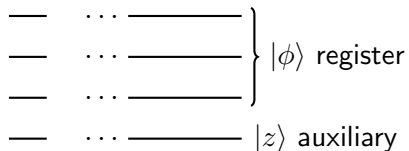
$$\left. \begin{array}{c} \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \\ \text{---} \quad \dots \text{---} \end{array} \right\} |\phi\rangle \text{ register}$$
$$\text{---} \quad \dots \text{---} \quad |z\rangle \text{ auxiliary}$$

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

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

$|\phi_i\rangle$  corresponds to a single classical variable  $x_{i,t}^r$ .

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$$n_q = 1 + \log_2 n_c$$

## Example

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$$x^* = (1, 1, 1, 0)^\dagger$$

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

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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

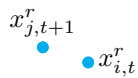
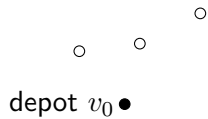


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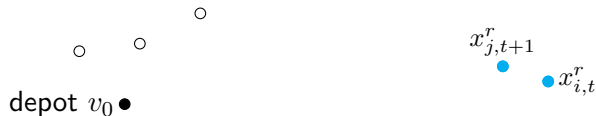


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$$|\psi(\theta)\rangle = \sum_{i=1}^{n_c} \beta_k(a_i|0\rangle + b_i|1\rangle) |\phi_i\rangle$$

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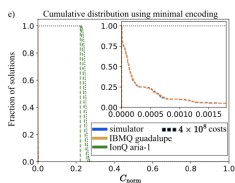
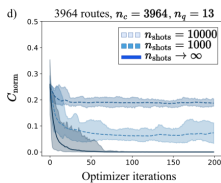
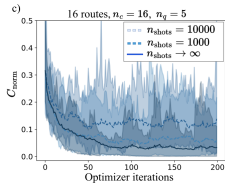
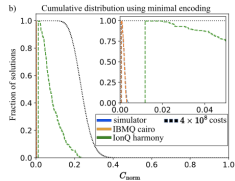
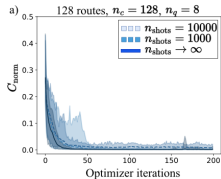
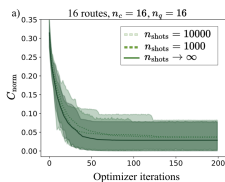


$$|\psi(\theta)\rangle = \sum_{i=1}^{n_c} \beta_k(a_i|0\rangle + b_i|1\rangle) |\phi_i\rangle$$

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]

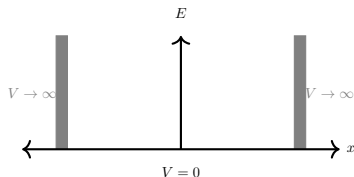
Thank you for your attention.

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



# Backup slides

## Adiabatic computation

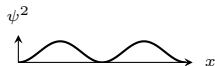


$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t)$$

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

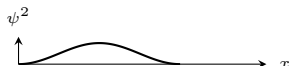
# Backup slides

## 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

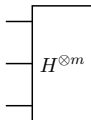
$$|\psi(\beta, \gamma)\rangle =$$

# Backup slides

QAOA

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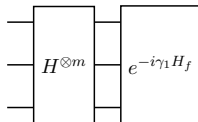
$$|+\rangle^{\otimes m}$$



# Backup slides

QAOA

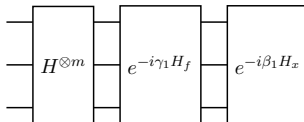
$$|\psi(\beta, \gamma)\rangle = e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$



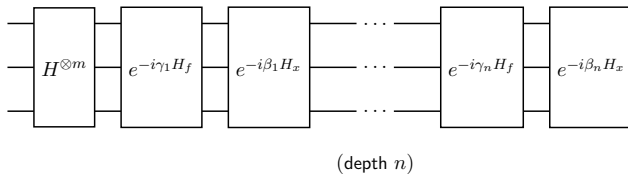
# Backup slides

QAOA

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



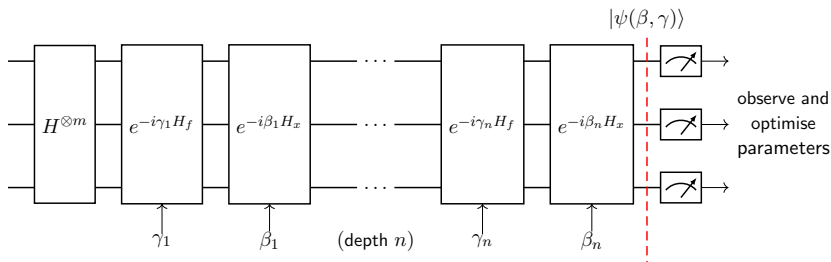
$$|\psi(\beta, \gamma)\rangle = \prod_k e^{-i\beta_k H_x} e^{-i\gamma_k H_f} |+\rangle^{\otimes m}$$



# Backup slides






## QAOA





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







# References I

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