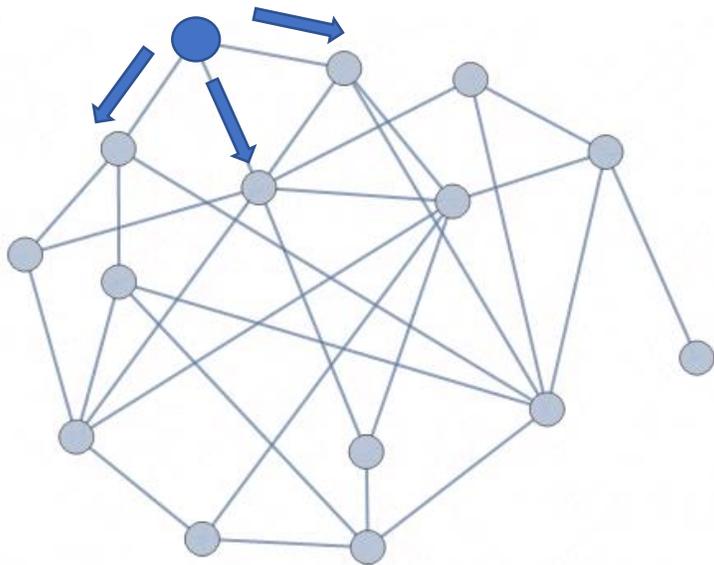


Quantum search and optimization using quantum walks

Leonardo Novo

Quantum and Linear-Optical Computation group
INL, Portugal

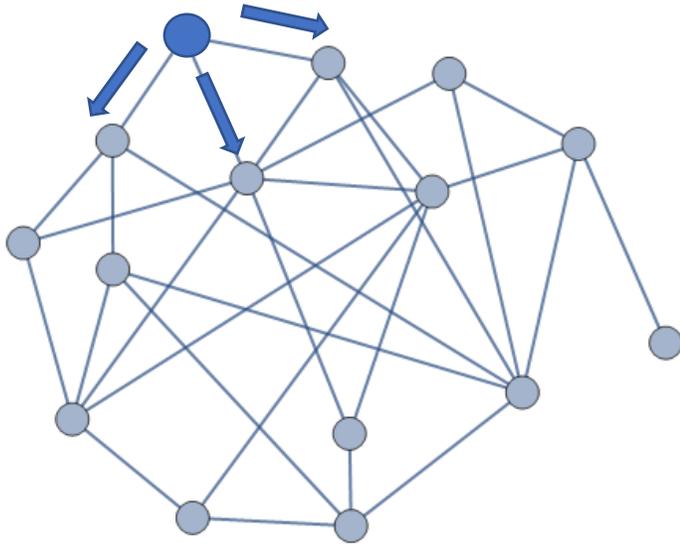


QuData workshop, 24 January 2024

Structure

- Continuous-time quantum walks
- Quantum search via continuous-time quantum walk: Childs and Goldstone approach
- Optimality and limitations
- Quantum walks for optimization (ongoing work)

Continuous-time classical random walk



Graph Laplacian:
 $L = D - A$

Encodes connectivity of graph

Degree matrix D :

$$D_{ii} = \deg(v_i)$$

Adjacency matrix A :

$$A_{ij} = \begin{cases} 1, & (i, j) \in E_G \\ 0, & \text{otherwise} \end{cases}$$

Differential equation describing the walk:

$$\frac{dp_j(t)}{dt} = -\gamma \sum_k L_{jk} p_k(t)$$

Real parameter (rate)

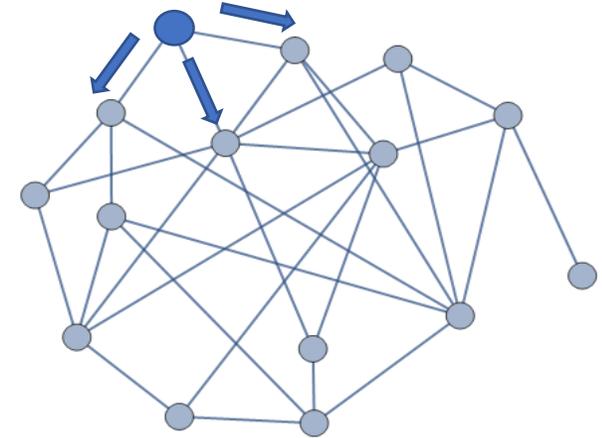
undirected graph $\Rightarrow L$ is symmetric

Continuous-time quantum walk

Schrödinger equation

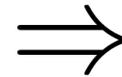
$$i \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

Idea: Choose Hamiltonian $H = \gamma L$



Differential equation describing the quantum walk:

$$\frac{d\alpha_j(t)}{dt} = -i\gamma \sum_k L_{jk} \alpha_k(t)$$



Time-evolution:

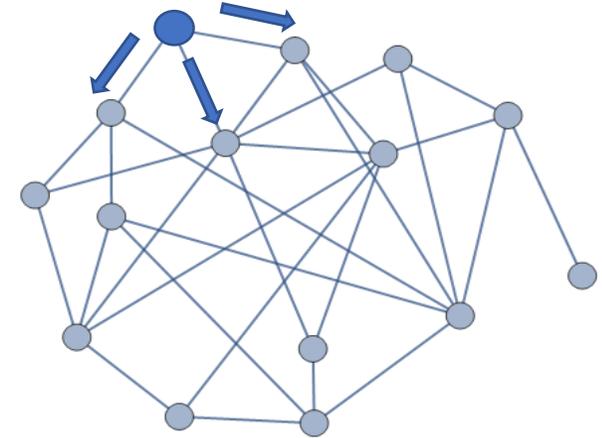
$$|\psi(t)\rangle = e^{-i\gamma L t} |\psi(0)\rangle$$

Continuous-time quantum walk

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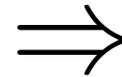
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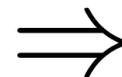
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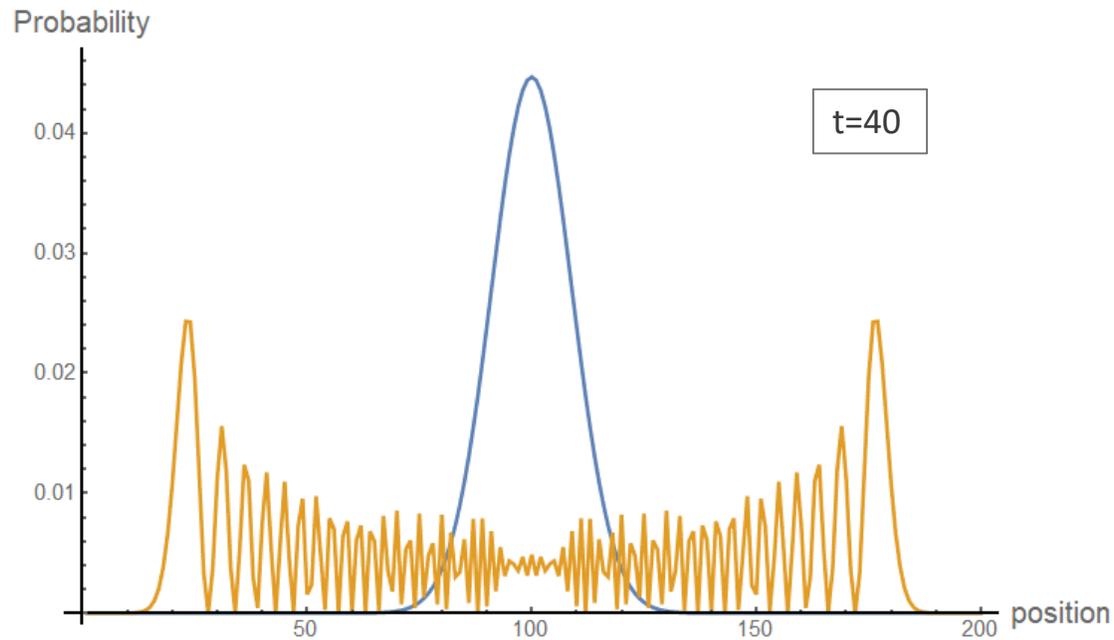
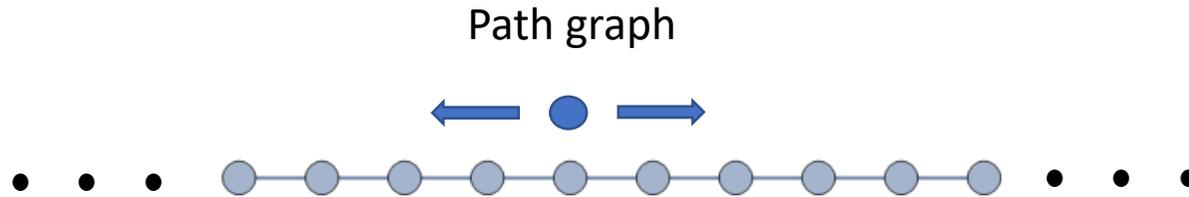
$$|\psi(t)\rangle = e^{-i\gamma L t} |\psi(0)\rangle$$

CTRW:
$$\frac{dp_j(t)}{dt} = -\gamma \sum_k L_{jk} p_k(t)$$



$$\vec{p}(t) = e^{-\gamma L t} \vec{p}(0)$$

Classical vs Quantum random walk



Quantum walk spreads **quadratically faster**

Standard deviation of position
after time t :

Classical walk

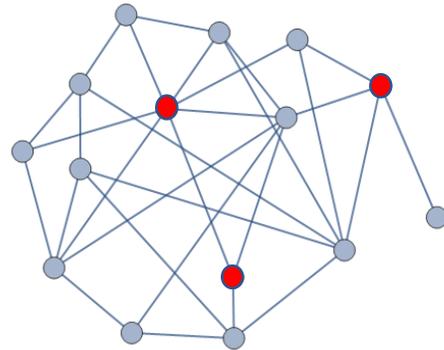
$$\sigma \propto \sqrt{t}$$

Quantum walk

$$\sigma \propto t$$

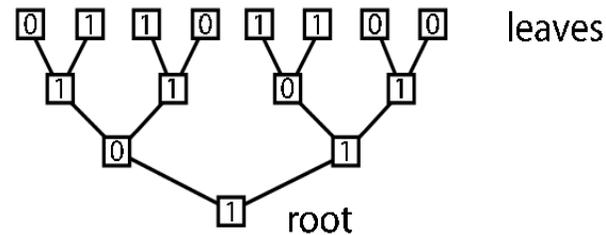
Applications of quantum walks

Search problems



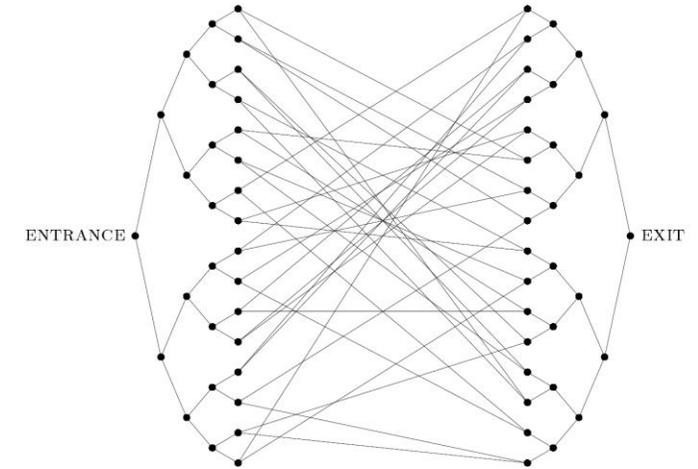
Childs, Andrew M., and Jeffrey Goldstone.
"Spatial search by quantum walk."
Physical Review A 70.2 (2004): 022314.

NAND trees



Farhi, Edward, Jeffrey Goldstone, and Sam
Gutmann. "A quantum algorithm for the
Hamiltonian NAND tree." *TOC 2008* .

Graph traversal problems



Childs, Andrew M., et al. "Exponential
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STOC 2003

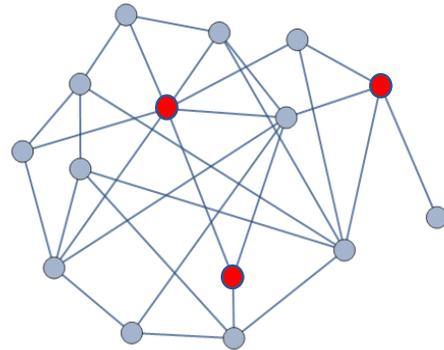
Gilyén, András, et al "(Sub) Exponential
advantage of adiabatic Quantum computation
with no sign problem.", *STOC 2021*

Others:

Element distinctness, triangle finding, ...

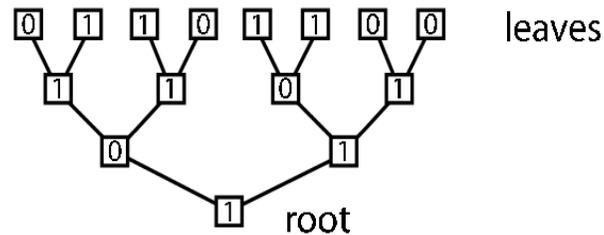
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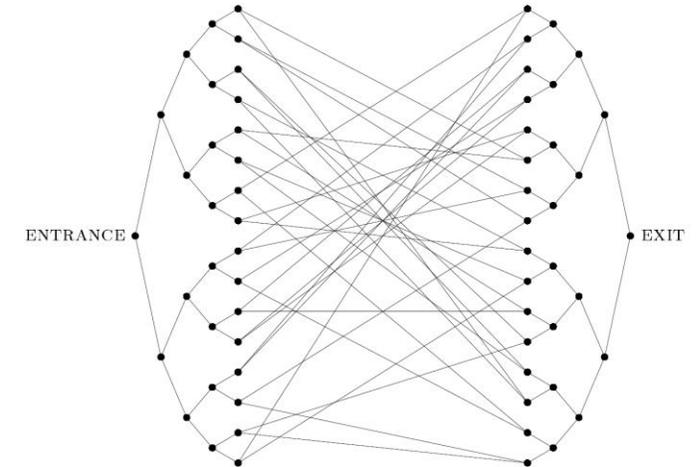
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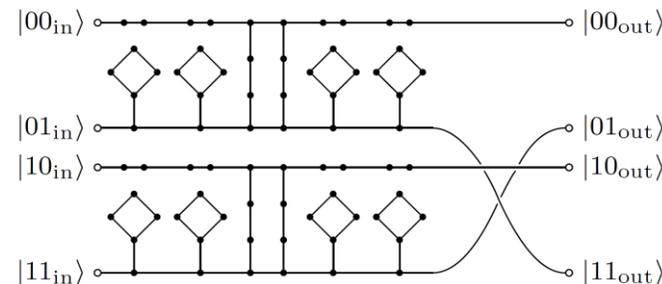
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Universal model of quantum computation



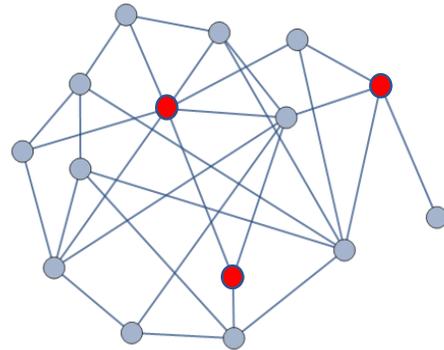
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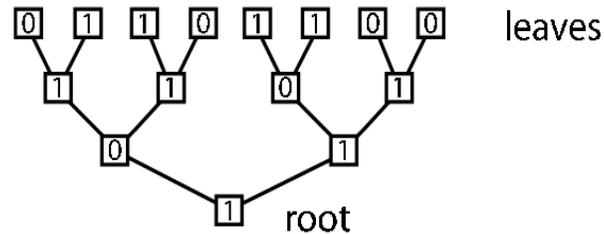
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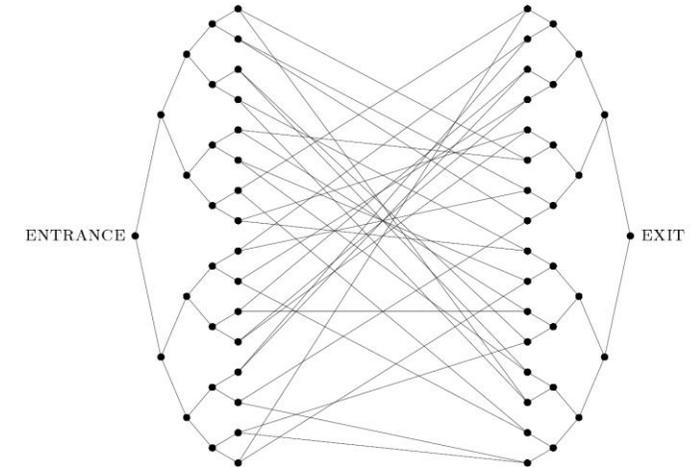
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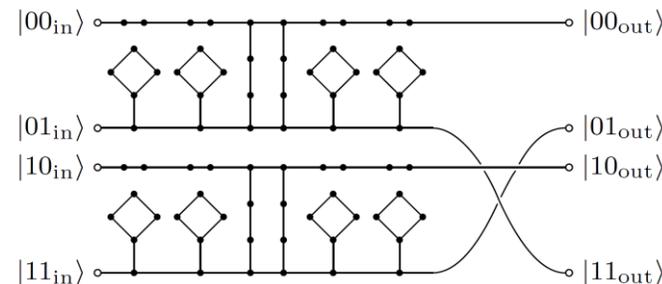
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Others:

Element distinctness, triangle finding, ...

Grover's algorithm for unstructured search

Construct Grover Oracle:

$$\begin{cases} U_w |w\rangle = -|w\rangle, \text{ if } w \text{ is the solution} \\ U_x |x\rangle = |x\rangle, \text{ otherwise} \end{cases}$$

Grover diffusion operator:

$$U_s = 2|s\rangle\langle s| - \mathbb{1}$$

Initial state:

$$|s\rangle = \frac{1}{\sqrt{n}} \sum_i |i\rangle = \frac{1}{\sqrt{n}} (1, 1, \dots, 1)$$

Algorithm:

$$(U_s U_w)^K |s\rangle, \text{ with } K = O(\sqrt{n})$$



Optimal!

Success Probability:

$$|\langle w | (U_s U_w)^K |s\rangle|^2 \approx 1$$

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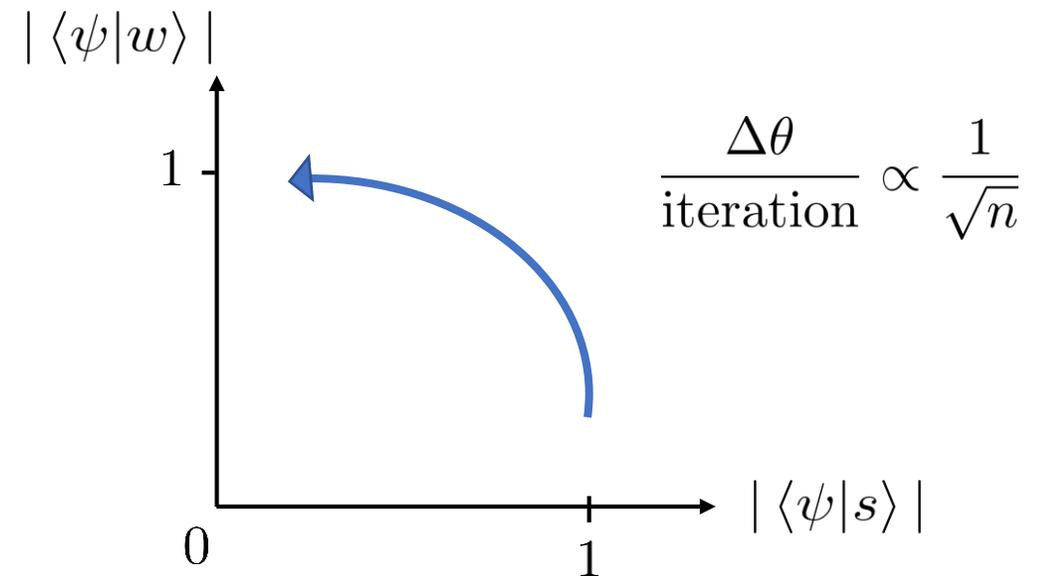
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Algorithm:

$$(U_s U_w)^K |s\rangle, \text{ with } K = O(\sqrt{n}) \rightarrow \text{Optimal!}$$

Success Probability:

$$|\langle w | (U_s U_w)^K |s\rangle|^2 \approx 1$$



Generates rotation in 2d subspace $\{|w\rangle, |s\rangle\}$

An analog analogue of Grover's algorithm (Farhi, Gutmann 98)

Solving a search problem via continuous-time evolution:

$$i \frac{d}{dt} |\psi\rangle = H |\psi\rangle = (H_O + H_D) |\psi\rangle$$

With the oracle Hamiltonian

$$H_O = |w\rangle\langle w|$$

Task: Find $|w\rangle$

Note that
 $e^{i\pi H_O} = U_w$

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Note that
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Task: Find $|w\rangle$

Solution: Add a driving term

$$H_D = |s\rangle\langle s|$$

Grover's algorithm

$$\prod_k e^{i\pi H_O} e^{i\pi H_D}$$

with $|s\rangle = \frac{1}{\sqrt{n}} \sum_i |i\rangle$

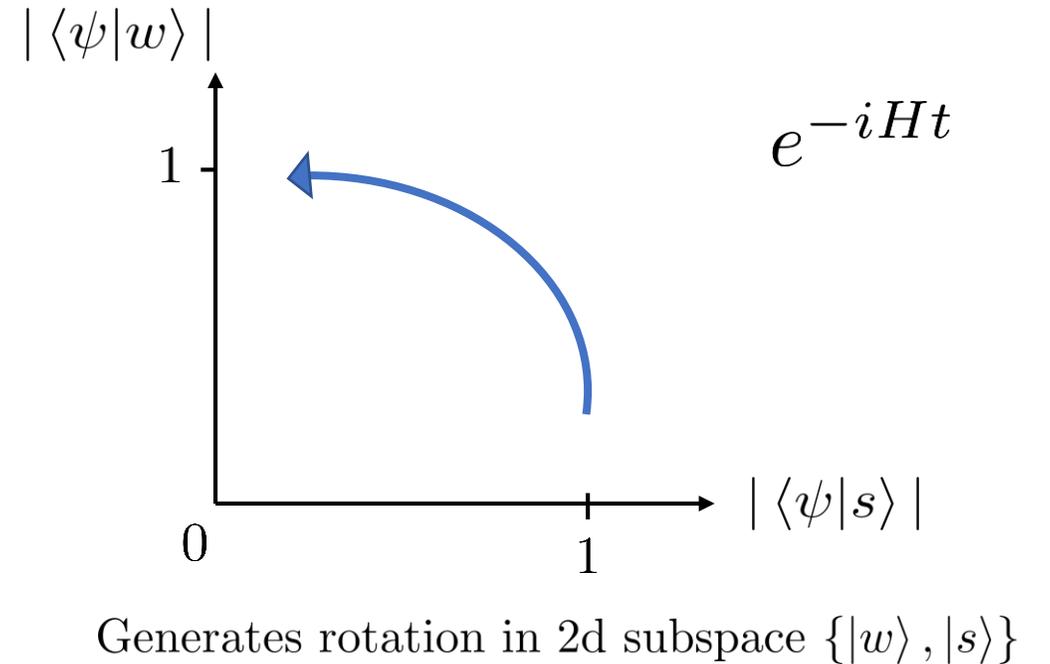
$$H = |w\rangle\langle w| + |s\rangle\langle s|$$

Generates rotation in 2d subspace $\{|w\rangle, |s_{\bar{w}}\rangle\}$

$$H = \begin{bmatrix} 1 & 1/\sqrt{n} \\ 1/\sqrt{n} & 1 \end{bmatrix} + O(1/n)$$

with $|s_{\bar{w}}\rangle = \frac{1}{\sqrt{n}} \sum_{i \neq w} |i\rangle$

Finds $|w\rangle$ after time $T = \Theta(\sqrt{n}) \rightarrow$ **Optimal!**



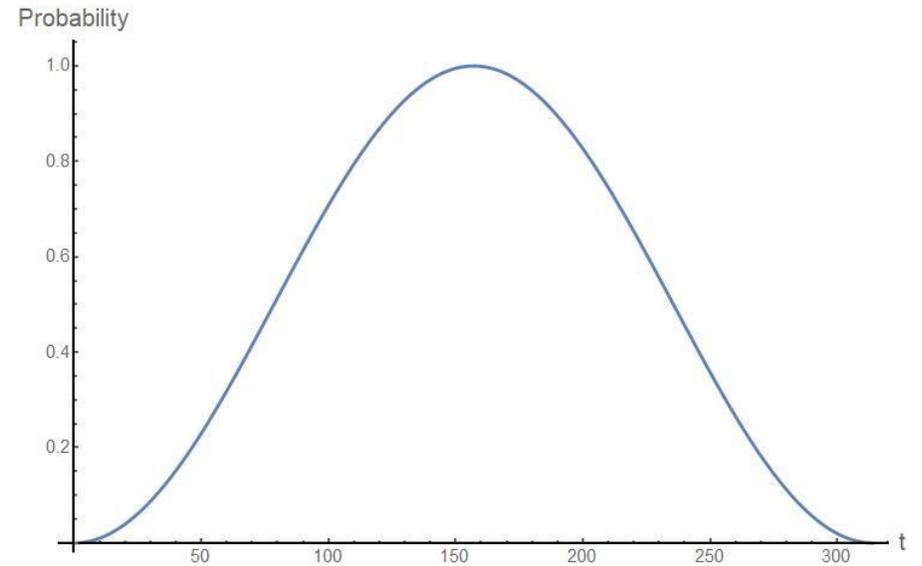
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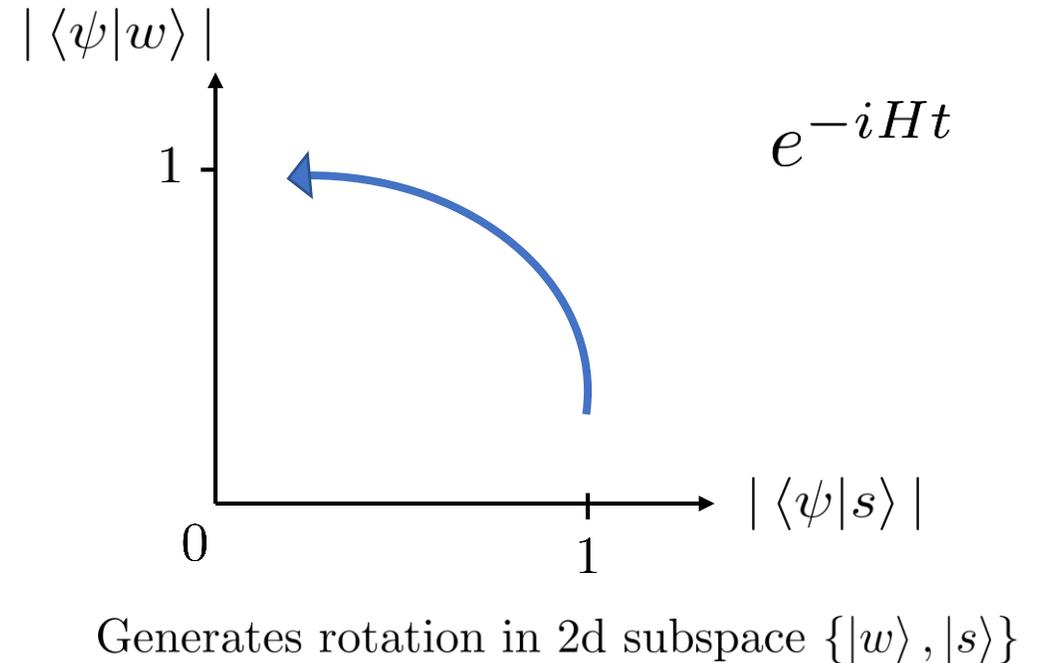
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Finds $|w\rangle$ after time $T = \Theta(\sqrt{n}) \rightarrow$ **Optimal!**



Matches lower bound on running time for any Hamiltonian of the form

$$H(t) = |w\rangle\langle w| + H_D(t)$$

Adiabatic quantum search

Adiabatic quantum computing:

- i) Start in ground state of Hamiltonian H_I .
- ii) Slowly change Hamiltonian towards a H_F .

$$H(t) = (1 - r(t))H_I + r(t)H_F$$

Adiabatic Theorem: If process is done *slowly enough*, the *ground state* of H_F is prepared with *high fidelity*.

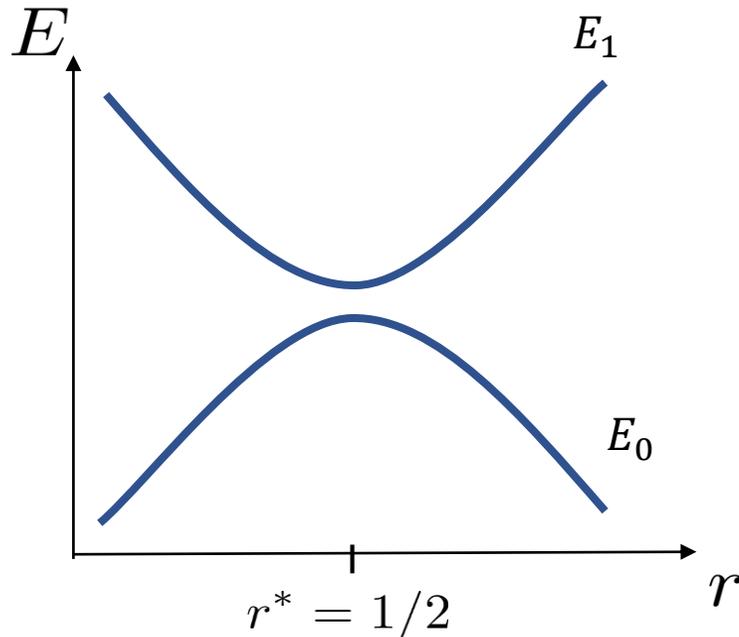
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Adiabatic Theorem: If process is done *slowly enough*, the ground state of H_F is prepared with *high fidelity*.



$$H(r) = -(1 - r)|s\rangle\langle s| - r|w\rangle\langle w|$$

- To get the optimal running time of $O(\sqrt{n})$, we need to adapt the *adiabatic schedule* $r(t)$.
- Linear schedule doesn't work! We need to go *slowly close to the minimum gap* and *fast elsewhere*.

Roland, Jérémie, and Nicolas J. Cerf. "Quantum search by local adiabatic evolution." *Physical Review A* 65.4 (2002): 042308.

What I talked about so far...

- Continuous-time quantum walks
- Grover's algorithm (circuit model)
- Farhi Gutmann algorithm (analog Grover, time-independent Hamiltonian)
- Adiabatic Grover algorithm (time-dependent Hamiltonian)

Coming up next...

- Search by quantum walk
- Optimization using quantum walks

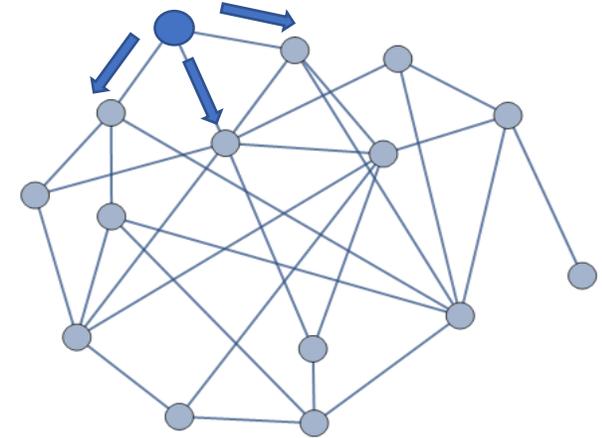
Part I: Quantum search using continuous-time quantum walks

Continuous-time quantum walk

Schrödinger equation

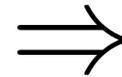
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Idea: Choose Hamiltonian $H = \gamma L$



Differential equation describing the quantum walk:

$$\frac{d\alpha_j(t)}{dt} = -i\gamma \sum_k L_{jk} \alpha_k(t)$$



Time-evolution:

$$|\psi(t)\rangle = e^{-i\gamma L t} |\psi(0)\rangle$$

Childs and Goldstone approach (spatial search)

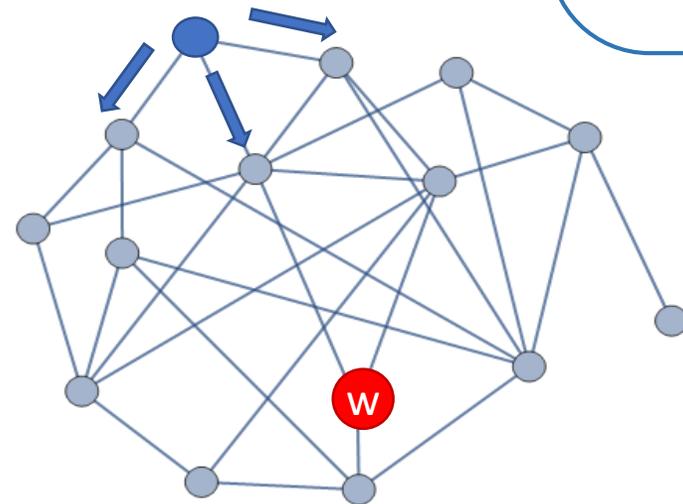
$$H = |w\rangle\langle w| + \gamma L$$

$$H_O = |w\rangle\langle w|$$

L graph's Laplacian \longrightarrow Or adjacency matrix

$|w\rangle$ marked state

γ real parameter (hopping rate)



$$L = D - A$$

Degree matrix D :

$$D_{ii} = \text{deg}(v_i)$$

Adjacency matrix A :

$$A_{ij} = \begin{cases} 1, & (i, j) \in E_G \\ 0, & \text{otherwise} \end{cases}$$

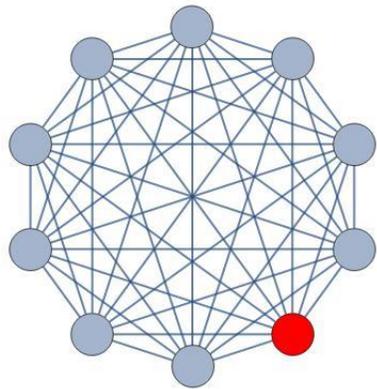
Starting from $|\psi(t=0)\rangle = |s\rangle$, and tuning γ carefully:

Complete graph

$$A_{ij} = 1$$

Choose $\gamma = 1/n$

$$\begin{aligned} H &= |w\rangle\langle w| + \frac{1}{n}A \\ &= |w\rangle\langle w| + |s\rangle\langle s| \end{aligned}$$

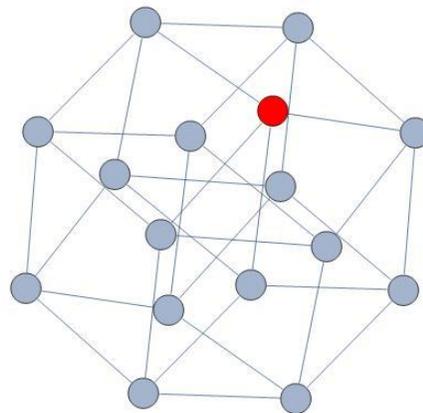


$$T = O(\sqrt{n}) \quad \text{Optimal!}$$

Hypercube

$$T = O(\sqrt{n})$$

Optimal!



Lattices

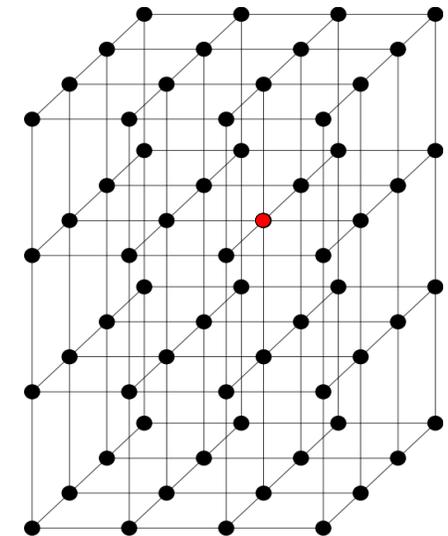
- $d \leq 3$: No significant speed-up

- $d = 4$:

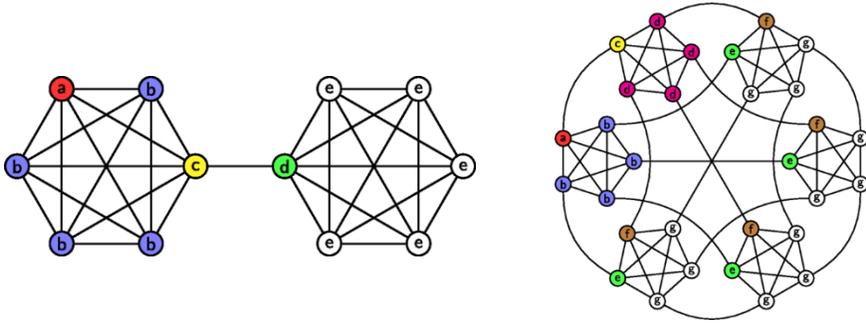
$$T = O(\sqrt{n} \log n)$$

- $d > 4$:

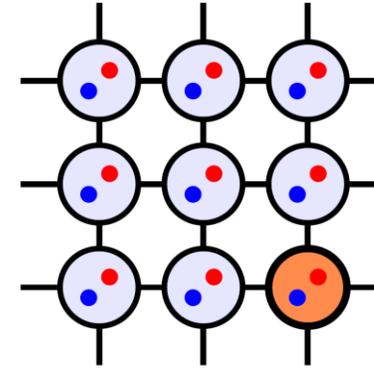
$$T = O(\sqrt{n}) \quad \text{Optimal!}$$



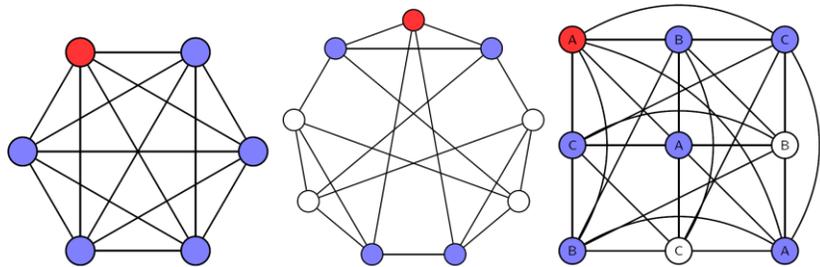
Subsequent work:



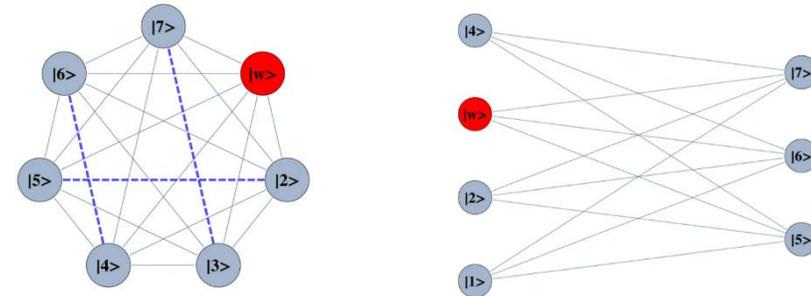
Meyer, David A., and Thomas G. Wong. "Connectivity is a poor indicator of fast quantum search." *Physical review letters* 114.11 (2015): 110503.



Andrew M. Childs and Yimin Ge. Spatial search by continuous-time quantum walks on crystal lattices. *Phys.Rev. A*, 89:052337, 2014



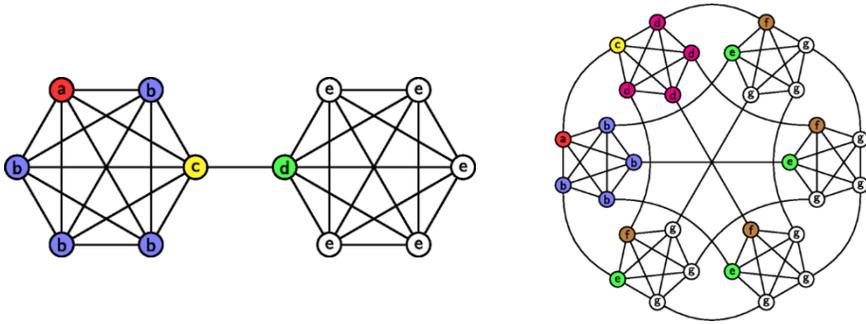
Jonatan Janmark, David A Meyer, Thomas G Wong. Global symmetry is unnecessary for fast quantum search. *Physical Review Letters*, 112(21):210502, 2014.



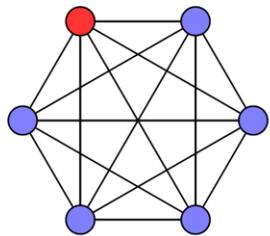
LN, et al. "Systematic dimensionality reduction for quantum walks: Optimal spatial search and transport on non-regular graphs." *Scientific reports* 5.1 (2015): 1-16.

and several others...

Subsequent work:



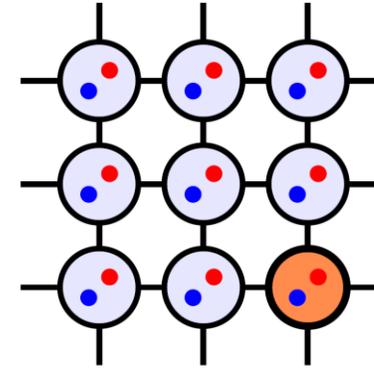
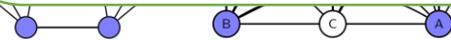
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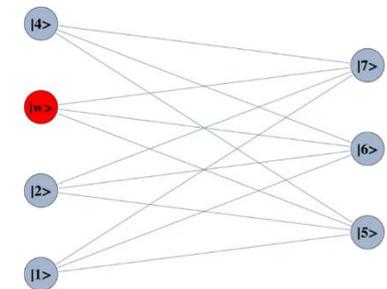
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Previous work: graph specific

Can we obtain general results about the performance of this search algorithm?



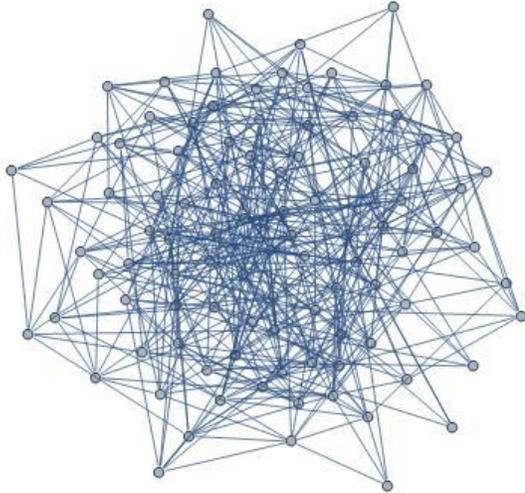
Yimin Ge. "Spatial search by quantum walks on crystal lattices." *Physical Review Letters* 109:052337, 2012.



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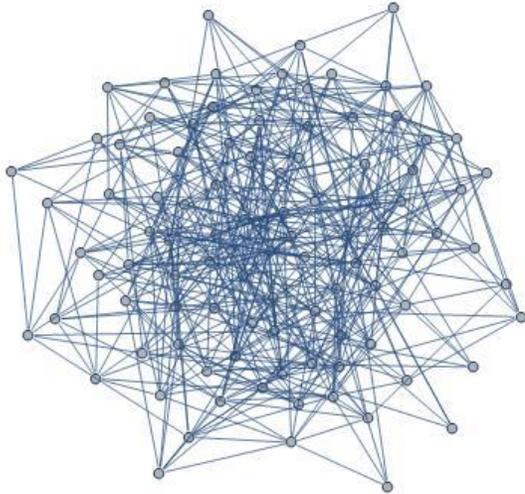
Quantum search on Erdős-Renyi random graphs $G(n, p)$



Shantanav Chakraborty, LN, Andris Ambainis, Yasser Omar. Spatial search by quantum walk is optimal for almost all graphs. Physical review letters, 116(10):100501, 2016.

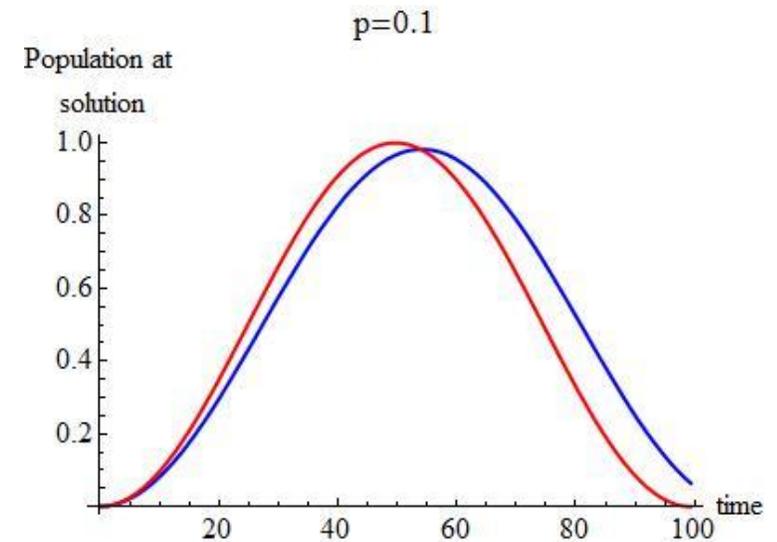
Two sites are connected with probability p

Quantum search on Erdős-Renyi random graphs $G(n, p)$

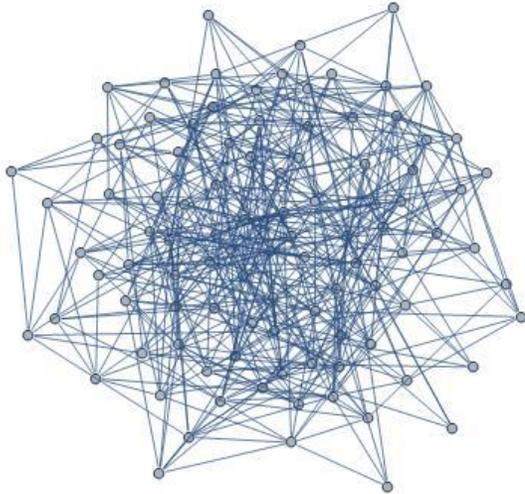


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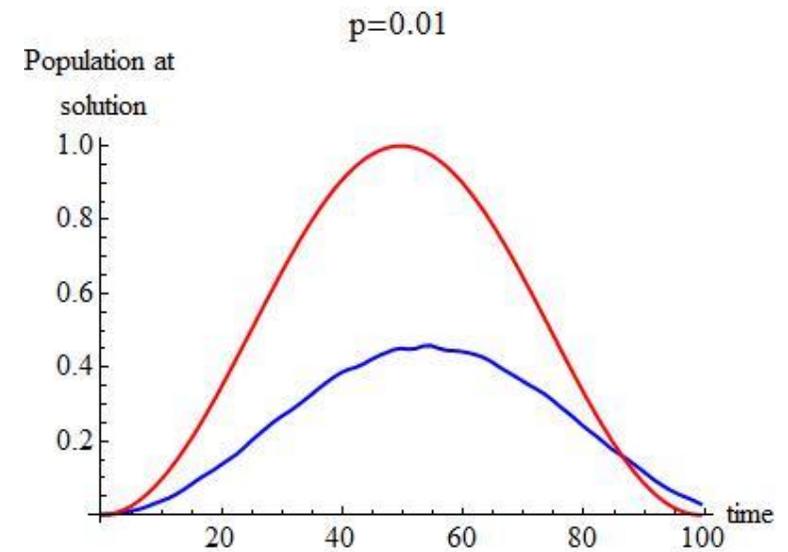


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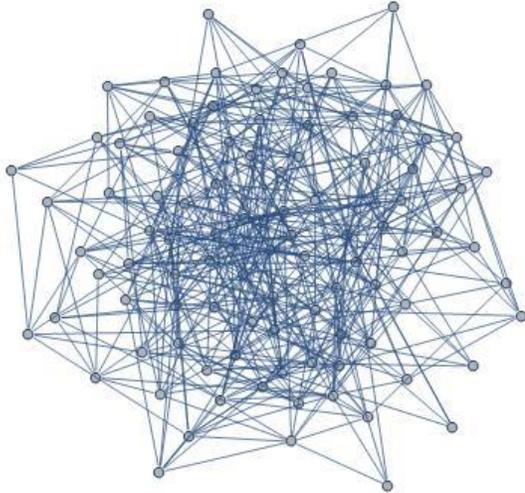


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Two sites are connected with probability p



Sufficient condition for optimal quantum search



Shantanav Chakraborty, LN, Andris Ambainis, Yasser Omar. Spatial search by quantum walk is optimal for almost all graphs. Physical review letters, 116(10):100501, 2016.

Graph Laplacian:

$$L = D - A$$



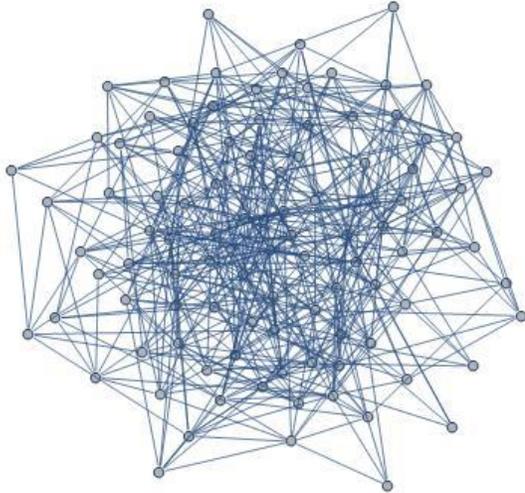
Normalized Laplacian:

$$L_{\text{norm.}} = \frac{L}{\lambda_{\max}}$$

Eigenvalues: $0 = \lambda'_1 < \lambda'_2 \leq \dots \leq \lambda'_n \leq 1$

Spectral gap: $\Delta = \lambda'_2 - \lambda'_1 = \lambda'_2$

Sufficient condition for optimal quantum search



Shantanav Chakraborty, LN, Andris Ambainis, Yasser Omar. Spatial search by quantum walk is optimal for almost all graphs. Physical review letters, 116(10):100501, 2016.

Graph Laplacian:

$$L = D - A$$



Normalized Laplacian:

$$L_{\text{norm.}} = \frac{L}{\lambda_{\max}}$$

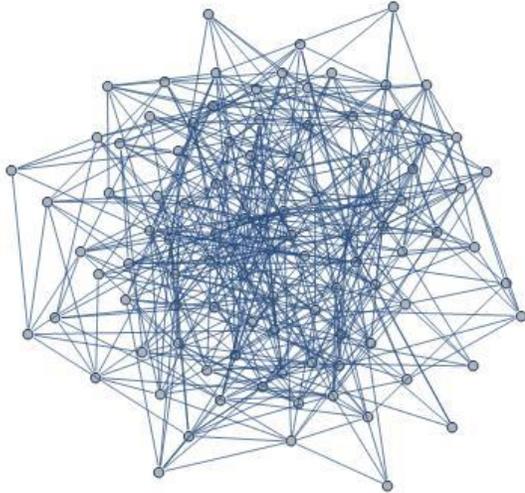
Eigenvalues: $0 = \lambda'_1 < \lambda'_2 \leq \dots \leq \lambda'_n \leq 1$

Spectral gap: $\Delta = \lambda'_2 - \lambda'_1 = \lambda'_2$

Constant Δ is a **sufficient condition** for optimal quantum search.

$$T = O(\sqrt{n}) \quad \text{Optimal!}$$

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$$p = \Omega\left(\frac{\log^{3/2} n}{n}\right)$$

Graph Laplacian:

$$L = D - A$$



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Optimality of spatial search via continuous-time quantum walk,
S. Chakraborty, L. Novo, Jérémie Roland, Phys. Rev. A 102, 032214, 2020

General results about performance for: $H_{\text{search}} = |w\rangle\langle w| + \gamma L_{\text{norm.}}$

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Notation

$$L_{\text{norm.}} = L/\lambda_{\text{max}}$$

Eigenvalues: $0 = \lambda'_1 < \lambda'_2 \leq \dots \leq \lambda'_n \leq 1$

Eigenvectors: $\{|v_i\rangle\}$

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We define: $S_k = \sum_{i>1} \frac{|\langle w|v_i\rangle|^2}{(\lambda'_i)^k}$

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We define: $S_k = \sum_{i>1} \frac{|\langle w|v_i\rangle|^2}{(\lambda'_i)^k}$

Condition on spectrum of L_{norm} (simplified)

$$\text{If } \Delta = \Omega(1/\sqrt{n})$$

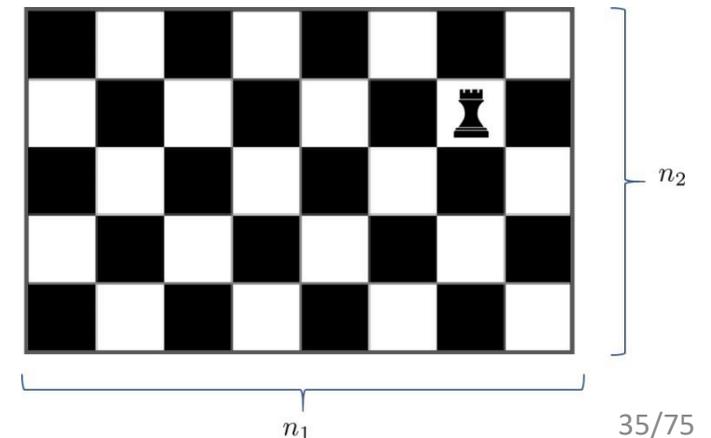
Performance of quantum search

- Best choice for γ : $\gamma = S_1$
- Best choice for evolution time: $T = \Theta\left(\frac{\sqrt{S_2}}{S_1} \sqrt{n}\right)$
- Success probability: $\Theta\left(\frac{S_1^2}{S_2}\right)$

Optimality of spatial search via continuous-time quantum walk,
S. Chakraborty, L. Novo, Jérémie Roland, Phys. Rev. A 102, 032214, 2020

- Provided **certain spectral conditions on L** are satisfied, we can predict ***best possible performance*** of the algorithm .
- New **sufficient condition** for optimal quantum search which ***reproduced all previous examples of optimality***.
- There are graphs for which search via the Childs and Goldstone approach ***does not provide a quadratic speed-up*** wrt classical random walk (e.g. Rook's graph).

$$\frac{S_1^2}{S_2} = \Theta(1)$$



General algorithms based on Hamiltonian evolution or discrete-time quantum walks to *speed-up search problems* for *any Markov Chain* and *any number of marked elements*.

DTQW

Quadratic speedup for finding marked vertices by quantum walks, A Ambainis, A Gilyén, S Jeffery, M Kokainis,. In *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing* (pp. 412-424), 2020.

CTQW

Quadratic Speedup for Spatial Search by Continuous-Time Quantum Walk, S Apers, S Chakraborty, LN, and J Roland, Phys. Rev. Lett. 129, 160502 (2022)

Part II: Can we design optimization algorithms using continuous-time quantum walks?

Childs and Goldstone approach (from spatial search to optimization)

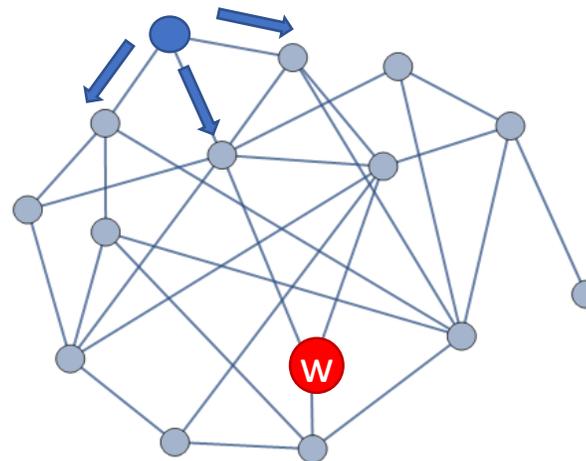
$$H = |w\rangle\langle w| + \gamma L \quad \longrightarrow \quad H = \sum_z f(z) |z\rangle\langle z| + \gamma L$$

L graph's Laplacian

$|w\rangle$ marked state

γ real parameter (hopping rate)

$$f(z) = \begin{cases} 1 & \text{if } z = w \\ 0 & \text{otherwise} \end{cases}$$



Can we use this kind of approach to optimize other cost functions?

Childs and Goldstone approach (from spatial search to optimization)

$$H = H_P + \gamma L$$

L graph's Laplacian

H_P problem Hamiltonian (site energies)

$$H_P = \sum_{i \neq j} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} + \sum_j h_j \sigma_z^{(j)}$$

γ real parameter (hopping rate)

**What can we prove about
speed-ups in this formalism?**

Childs and Goldstone approach (from spatial search to optimization)

$$H = H_P + \gamma L \quad \xrightarrow{\text{hypercube}} \quad H = H_P + \gamma L_{\text{hyp}}$$

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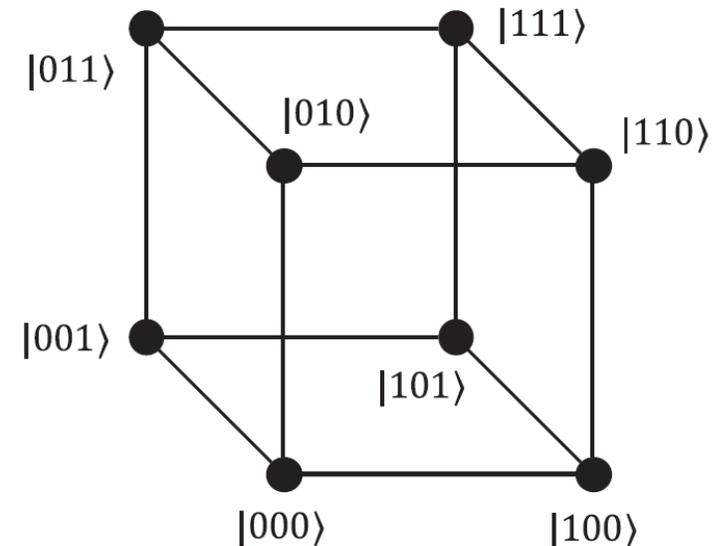
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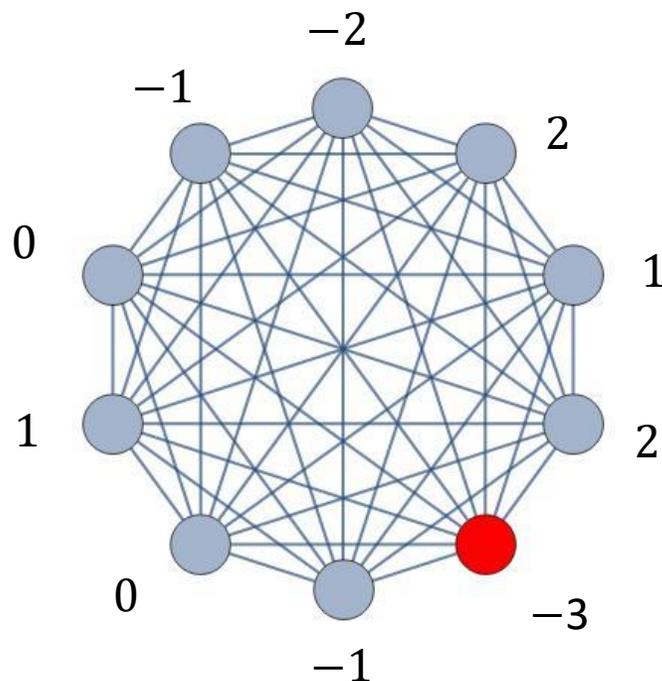


Part II A: Can we obtain provable quadratic speed-ups over classical unstructured search?

Optimization by CTQW on the complete graph

Complete graph:

$$H = H_P + \gamma L_{CG}$$
$$= H_P + \gamma' |s\rangle \langle s|$$



One-dimensional projector

Notice similarity with:

$$H_{\text{search}} = |w\rangle \langle w| + \gamma L_{\text{norm.}}$$

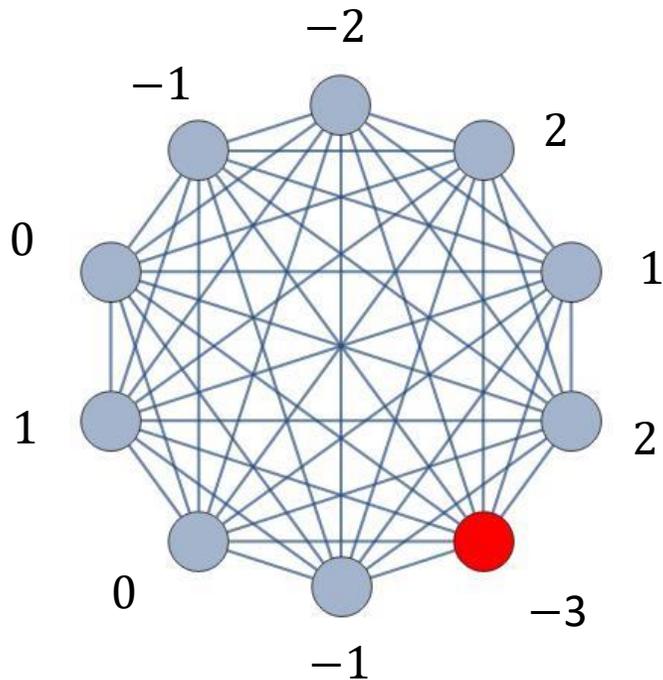
One-dimensional projector

We can use results from:

Optimality of spatial search via continuous-time quantum walk,
S. Chakraborty, L. Novo, Jérémie Roland, Phys. Rev. A 102, 032214, 2020

Optimization by CTQW on the complete graph

$$\begin{aligned} H &= H_P + \gamma L_{CG} \\ &= H_P + \gamma' |s\rangle \langle s| \end{aligned}$$



- Best choice for γ

$$\gamma^* = \frac{1}{N} \sum_{\alpha=1}^{M-1} \frac{d_{\alpha}}{E_{\alpha} - E_{GS}}$$

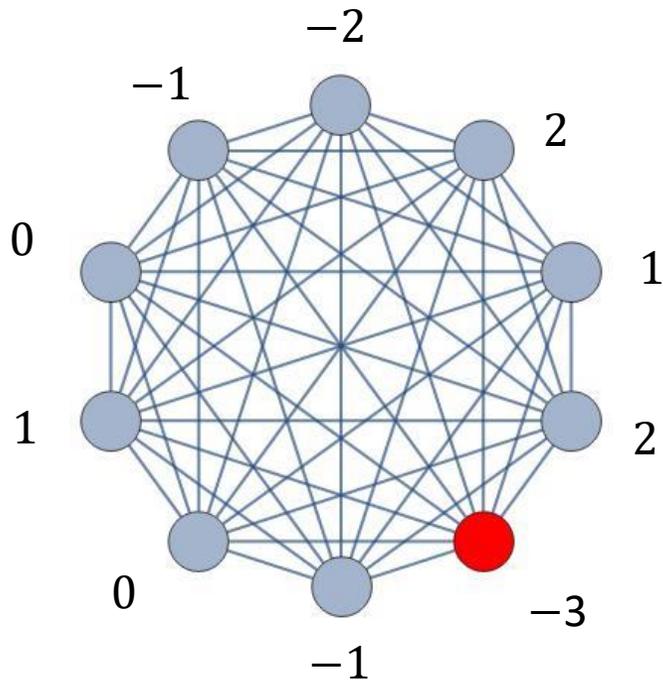
- E_{GS} - ground state energy of H_P
- E_{α} - other eigenvalues with degeneracy d_{α}

Running time:

$$T = O(\sqrt{N})$$

Optimization by CTQW on the complete graph

$$H = H_P + \gamma L_{CG}$$
$$= H_P + \gamma' |s\rangle \langle s|$$



Need to be
computed
beforehand. But
how??

- Best choice for γ

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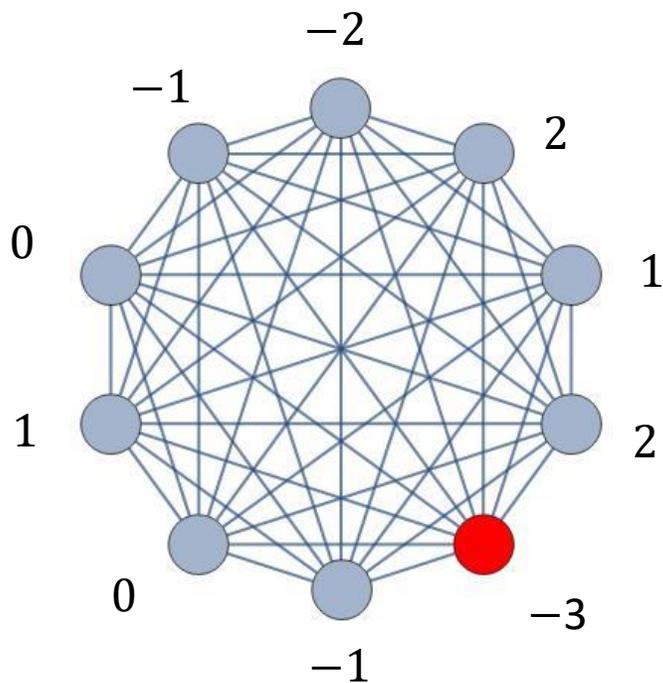
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For typical problem Hamiltonians (Ising)

$$H_P = \sum_{i \neq j} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} + \sum_j h_j \sigma_z^{(j)}$$

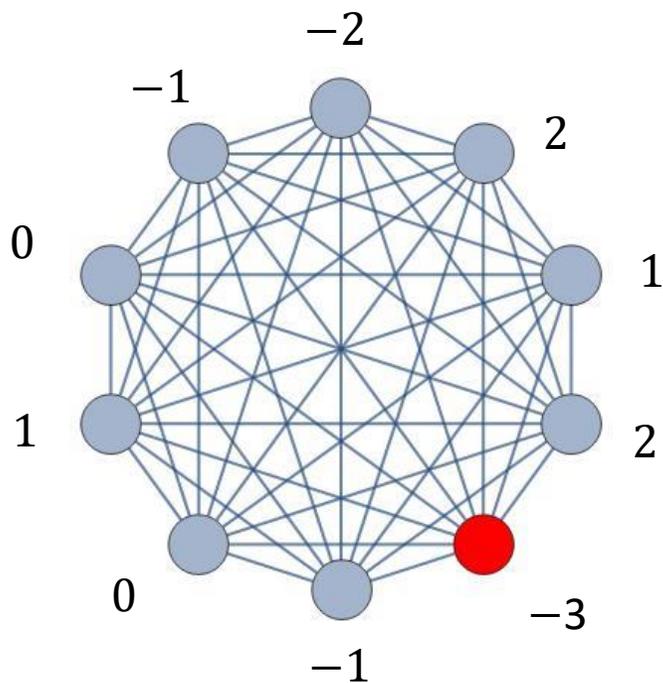
The problem of computing

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Is **#P-hard**

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The problem of computing

$$\gamma^* = \frac{1}{N} \sum_{\alpha=1}^{M-1} \frac{d_\alpha}{E_\alpha - E_{GS}}$$

Is **#P-hard**

Proof idea: Computing γ^* is as hard as computing amplitudes in IQP sampling.

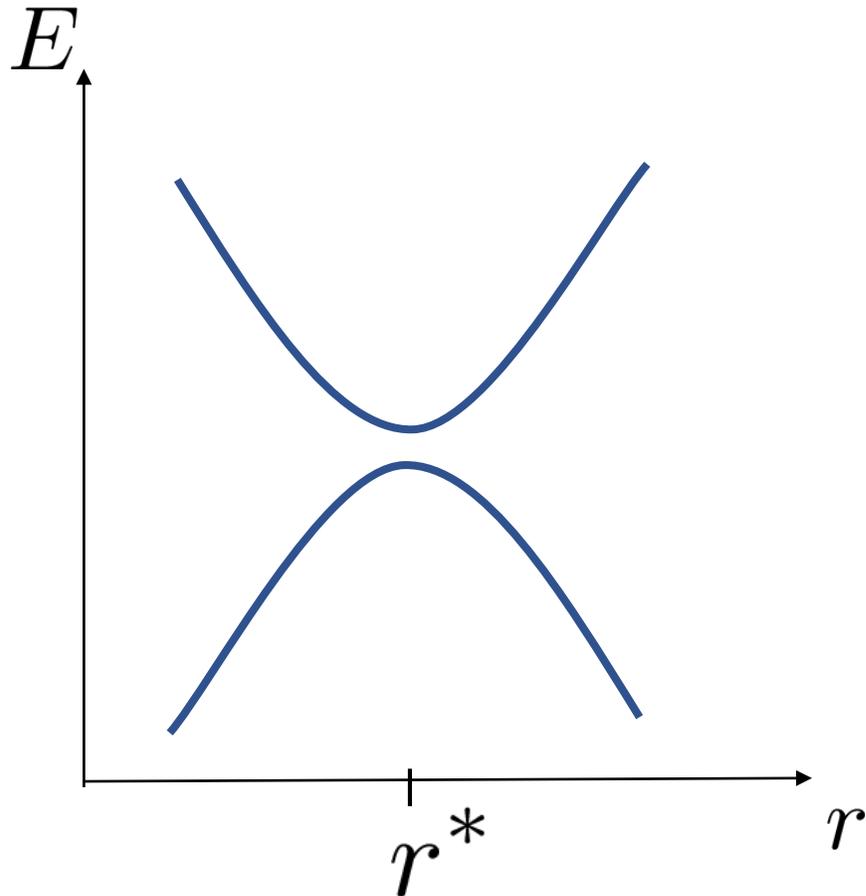
$$\langle s | e^{i \frac{\pi}{8} H_P} | s \rangle$$

Consequences for adiabatic quantum computing

$$H(r) = -(1 - r)|s\rangle\langle s| - rH_P$$

For Ising problems

$$H_P = \sum_{i \neq j} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} + \sum_j h_j \sigma_z^{(j)}$$



- Best possible running time: $O(\sqrt{N})$
- Achieving this running time needs knowledge about r^* .

J Roland, N Cerf "Quantum search by local adiabatic evolution." *PRA* (2002)

- **However**, computing r^* is a **#P-hard problem!**

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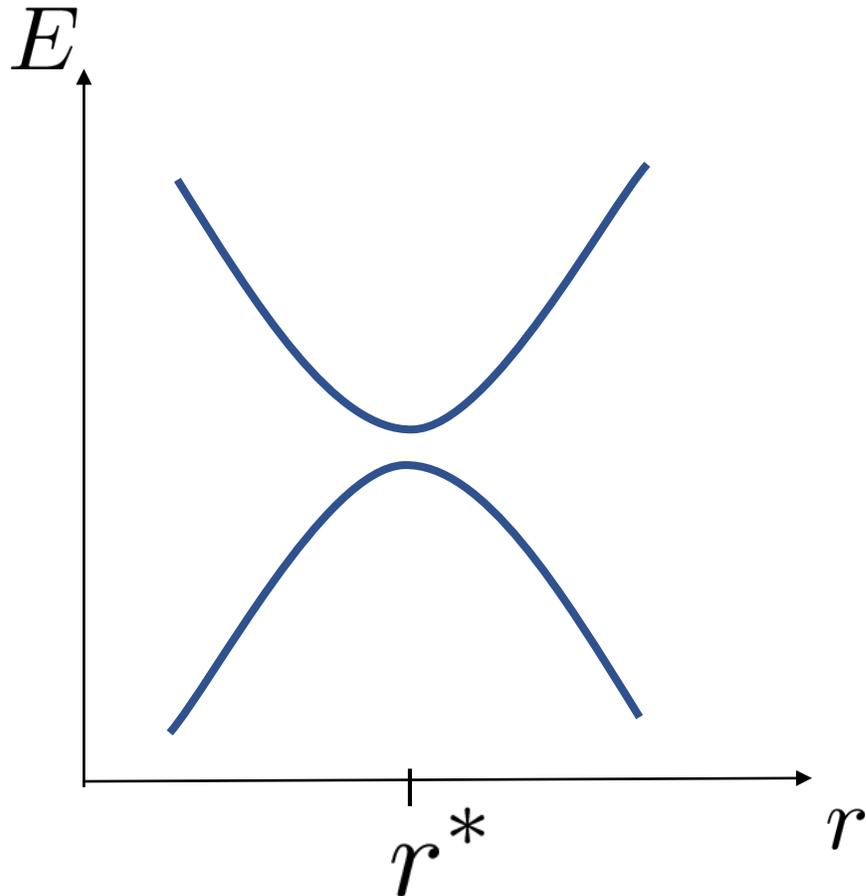
Already known:

- Best possible running time: $O(\sqrt{N})$
- Achieving this running time needs knowledge about r^* .

"How to make the quantum adiabatic algorithm fail"
E Farhi et al., *IJQI* (2008)

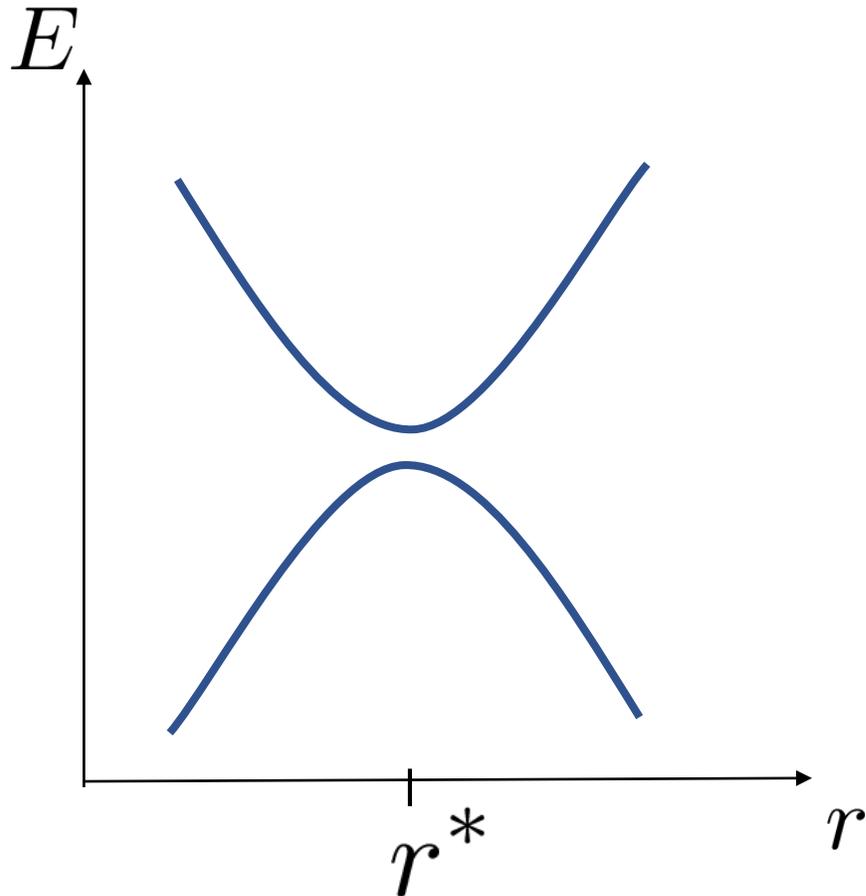
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- **However**, computing r^* is a **#P-hard problem!**



Consequences for adiabatic quantum computing

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Can adiabatic quantum computing provide **provable quadratic speed-ups** over unstructured search??

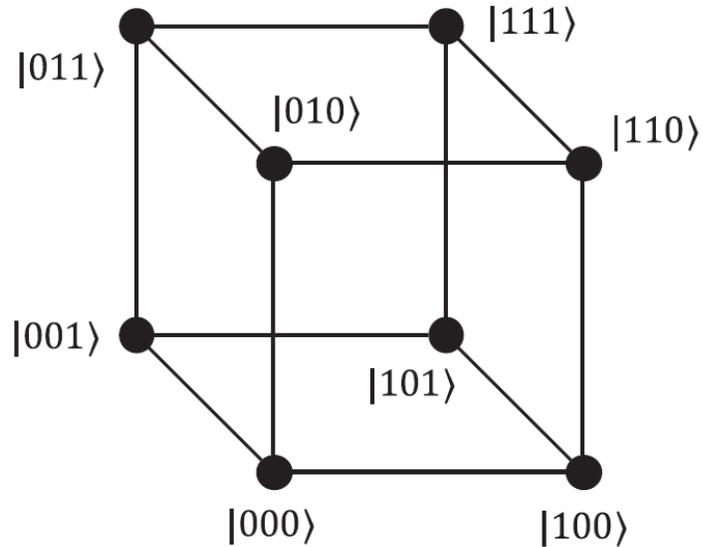
- **Some hope:** Computing r^* up to error $O\left(\frac{1}{\sqrt{N}}\right)$ should be enough.
- Can we do this in $O(\sqrt{N})$ time with a classical algorithm?
- Can we estimate it precisely enough by probing the quantum system?

Part II B: Heuristic quantum optimization algorithms using continuous-time quantum walks

Collaboration: Viv Kendon, Nicholas Chancellor,
Tamanna Dasanjh, Lasse Gerblich, Horatio Wong, David Ross

Optimization by CTQW on the hypercube

$$H = H_P + \gamma L_{\text{hyp}}$$
$$= H_P + \gamma \sum_j \sigma_x^{(j)}$$



Optimization by CTQW on the hypercube

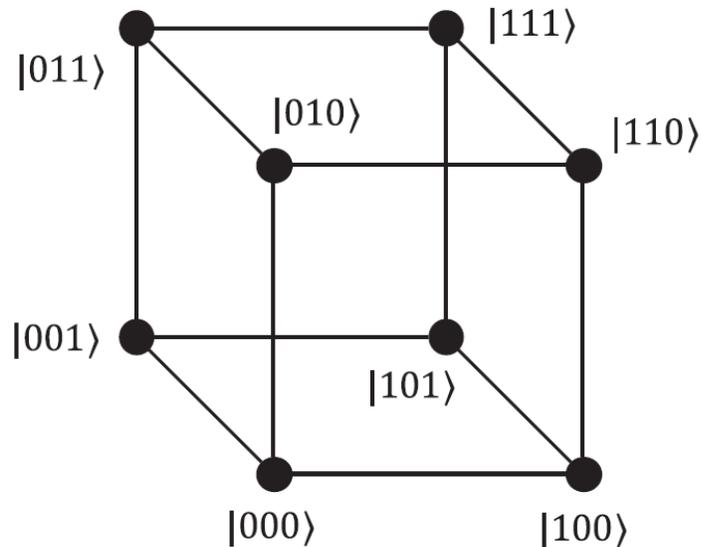
$$\begin{aligned} H &= H_P + \gamma L_{\text{hyp}} \\ &= H_P + \gamma \sum_j \sigma_x^{(j)} \end{aligned}$$

$$H_{SK} = - \sum_{j \neq k} J_{jk} \sigma_z^{(j)} \sigma_z^{(k)} - \sum_j h_j \sigma_z^{(j)}$$

$$J_{jk}, h_j \sim \mathcal{N}(0, \sigma^2)$$

**Sherrington-Kirkpatrick
model**

Adam Callison *et al* 2019 *New J. Phys.* **21** 123022



Optimization by CTQW on the hypercube

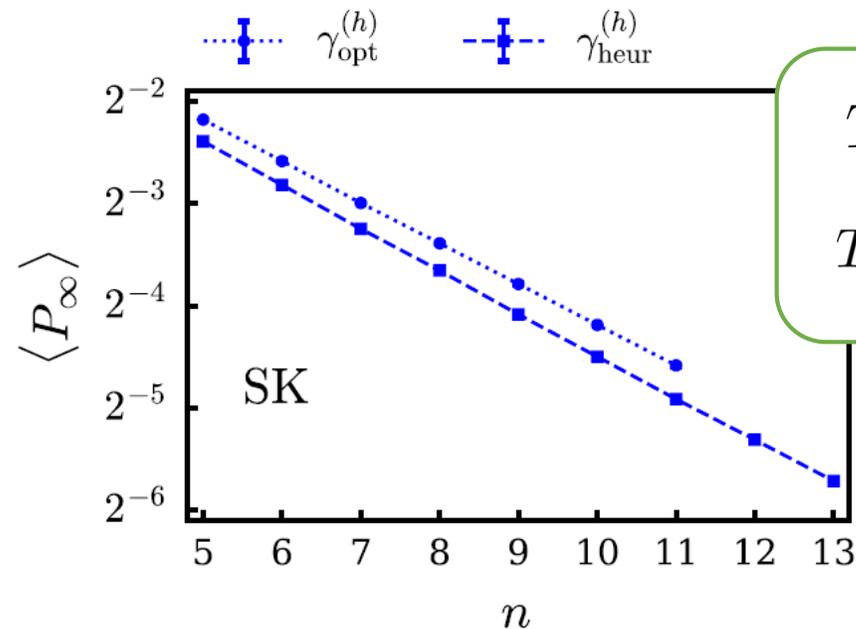
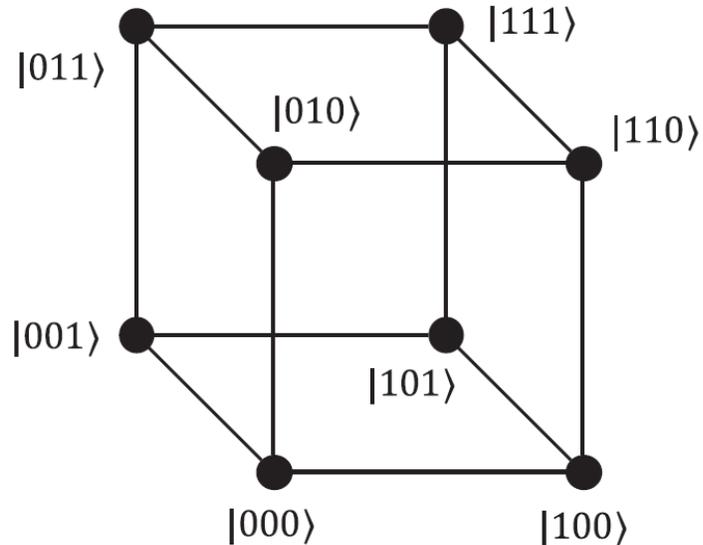
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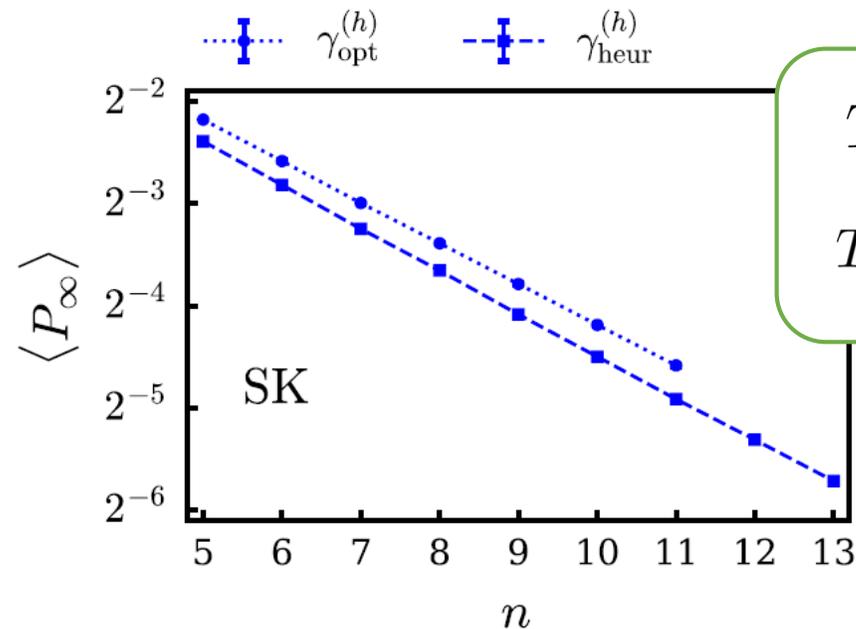
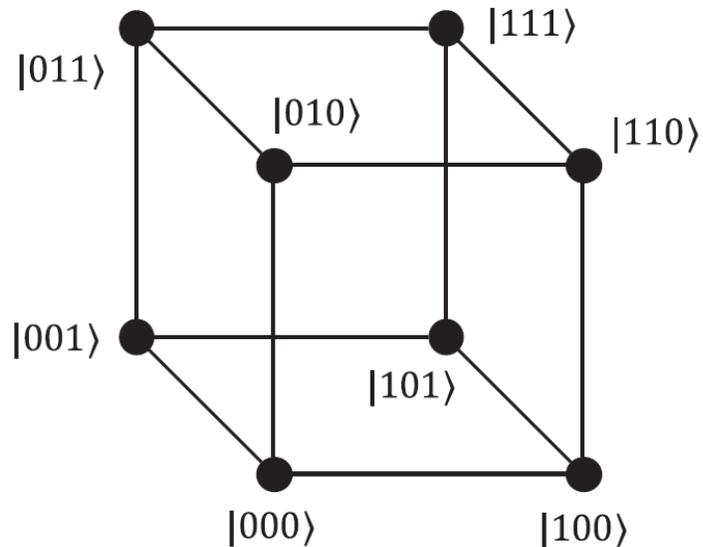
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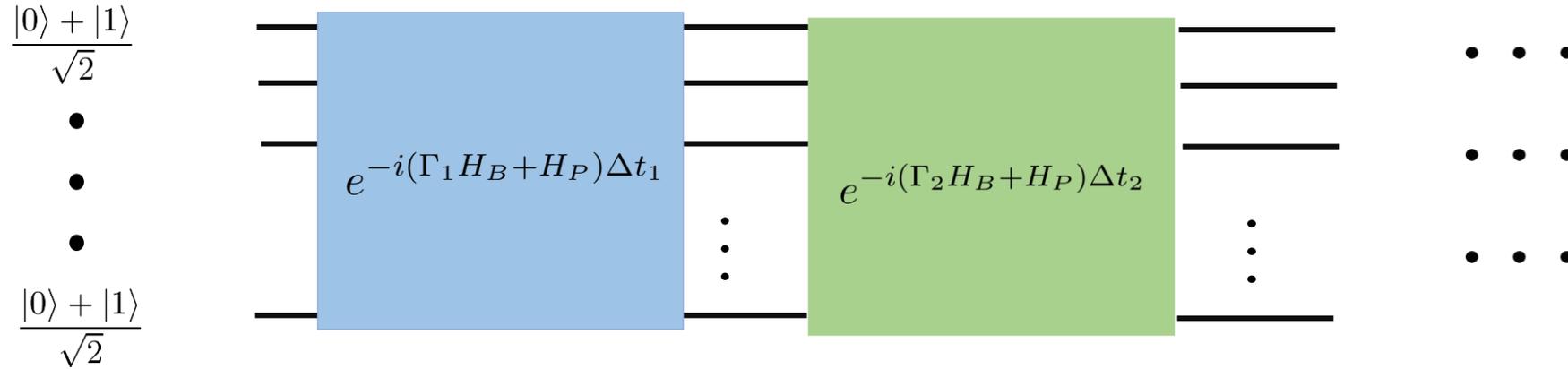
Adam Callison *et al* 2019 *New J. Phys.* **21** 123022



Better than Grover speed-up!

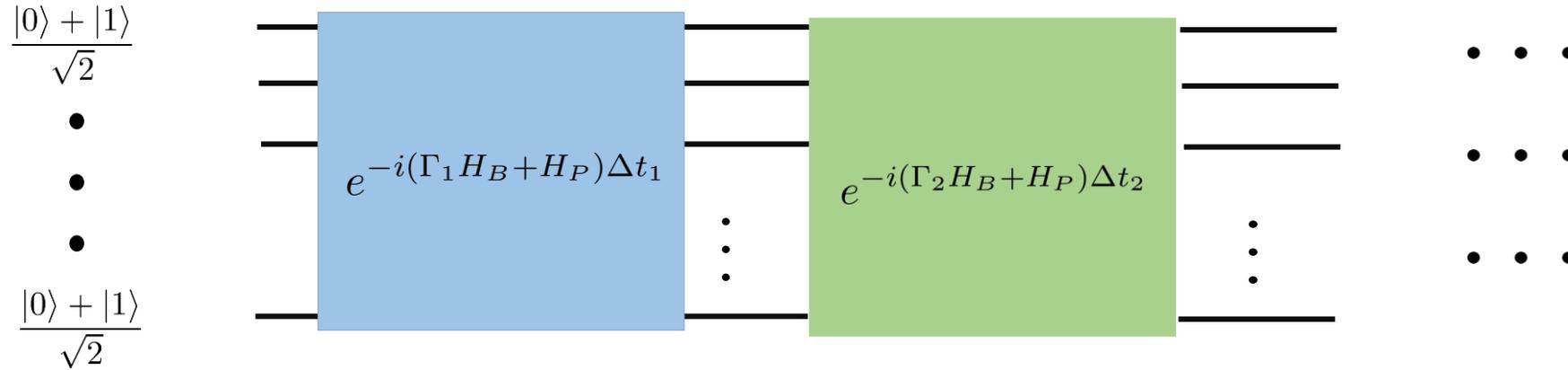
Multistage quantum walks:

$$H_B = - \sum_i \sigma_x^{(i)} \quad H_P = \sum_{i \neq j} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} + \sum_j h_j \sigma_z^{(j)}$$

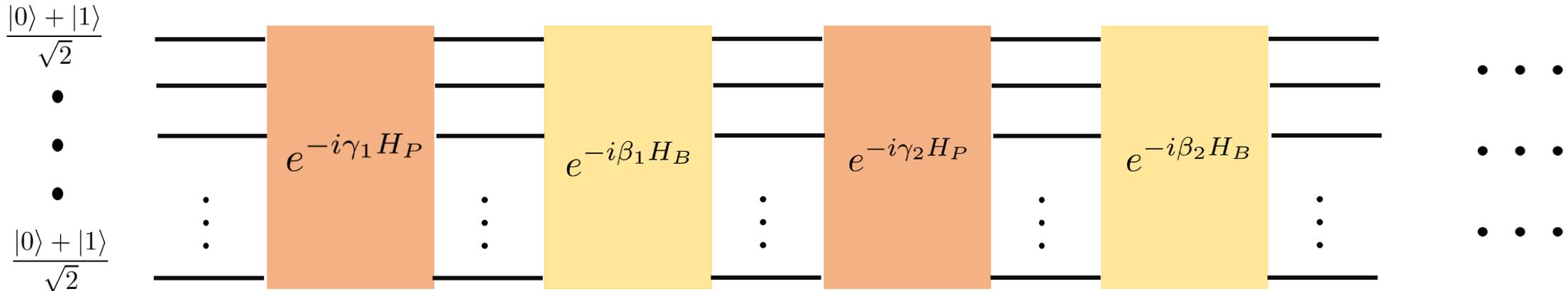


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QAOA:



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$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

•

•

•

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$



Two different *discretizations* of the *adiabatic algorithm*:

$$H(t) = (1 - r(t))H_B + r(t)H_P$$

Potential advantage: lower coherence times needed.

QAOA:

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

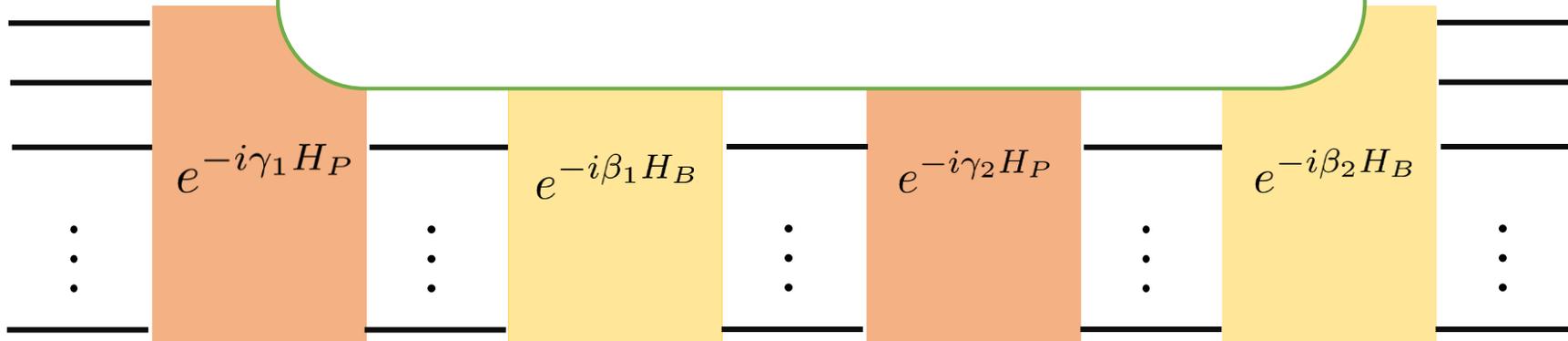
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⋮

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$



Multistage quantum walks VS QAOA

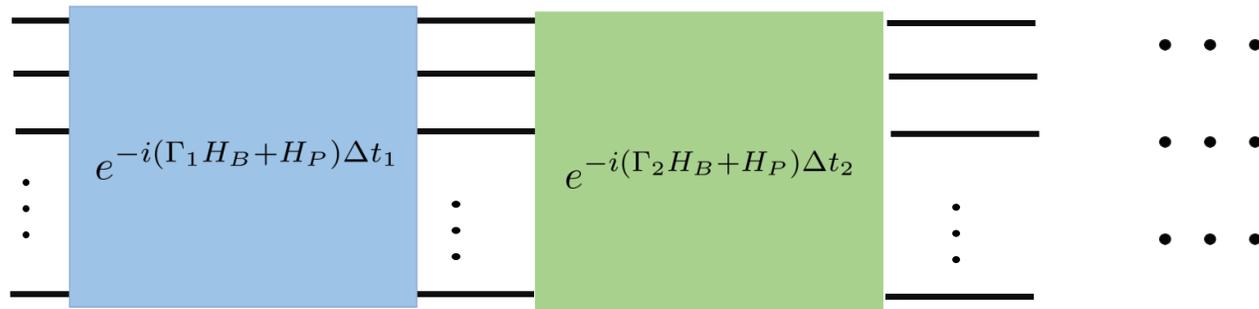
Quantum simulation: Discretization of evolution under time-dependent Hamiltonians

$$H(r(t)) = -(1 - r(t))H_B - r(t)H_P$$

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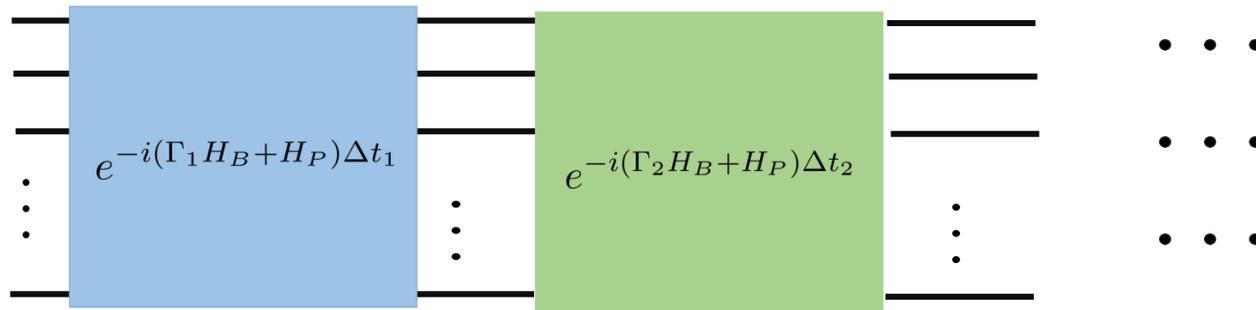
MSQW simulation error:

$$\epsilon_{td} \propto \dot{H}_{max}$$

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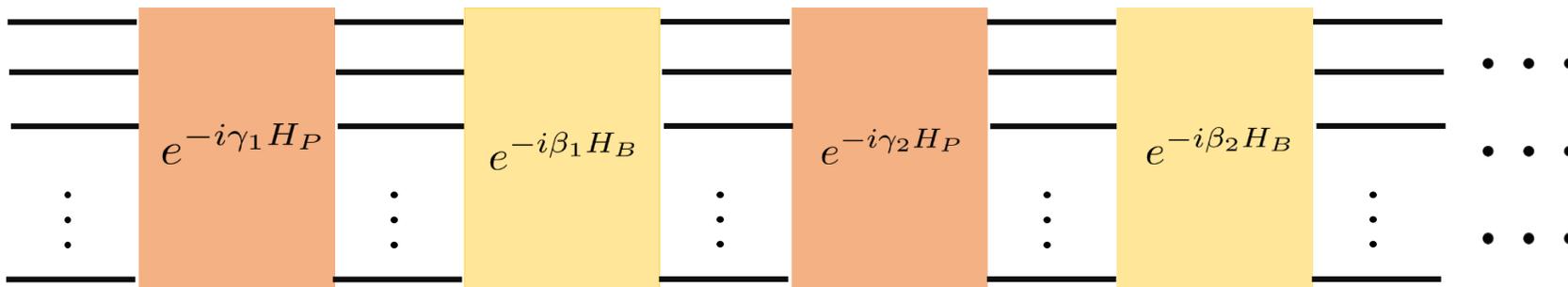
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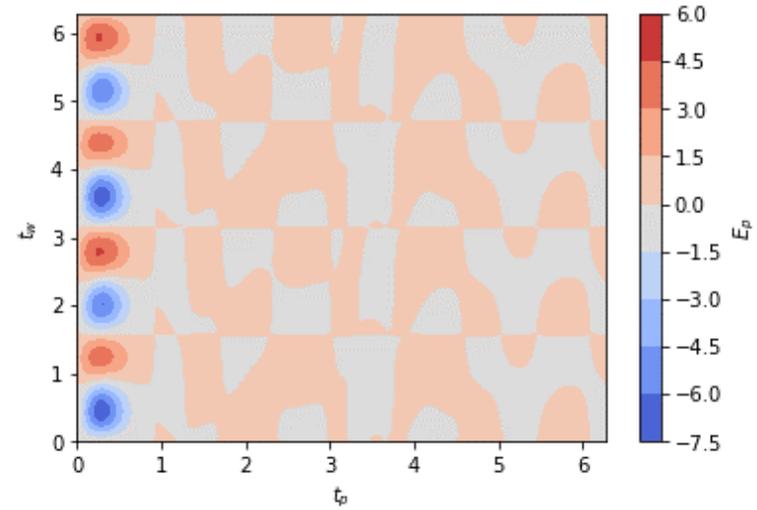
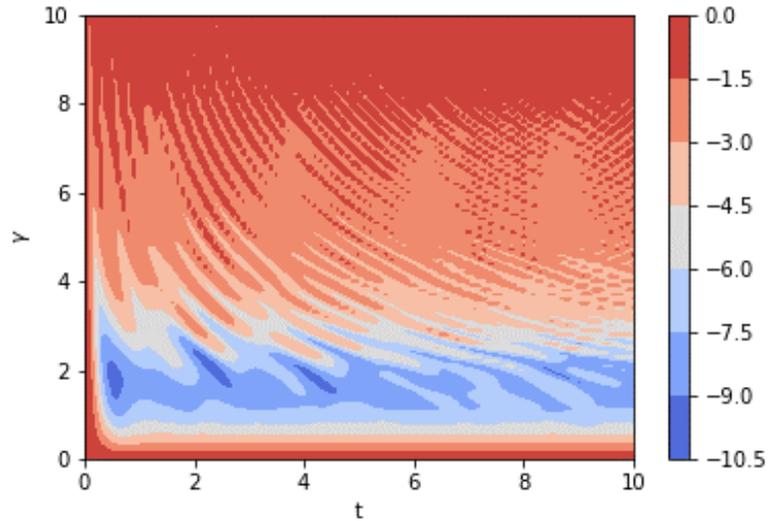
$$\epsilon_{total} = \epsilon_{td} + \epsilon_{Trotter}$$

Related to norms of commutators
between H_B and H_P

Multistage quantum walks VS QAOA

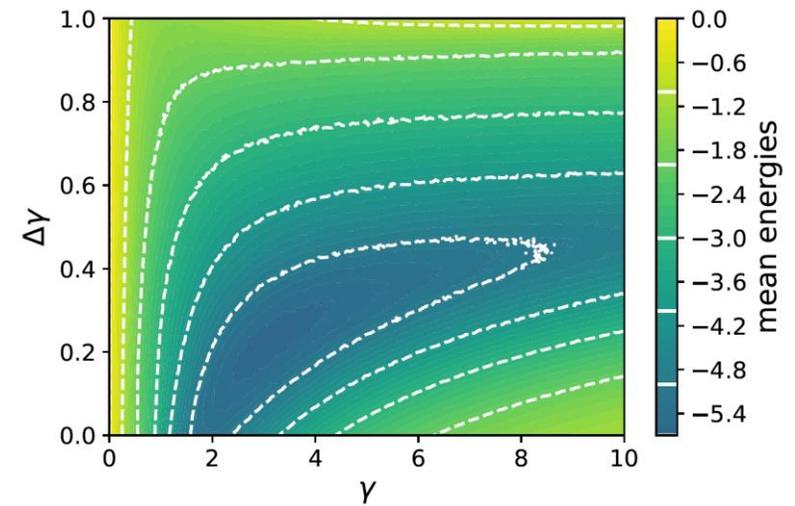
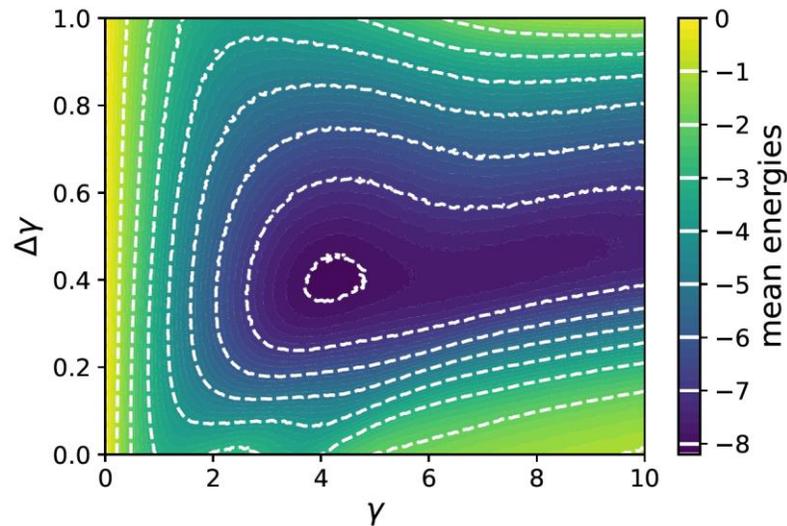
$$H_{QW} = \gamma H_B + H_P$$

Single-stage:



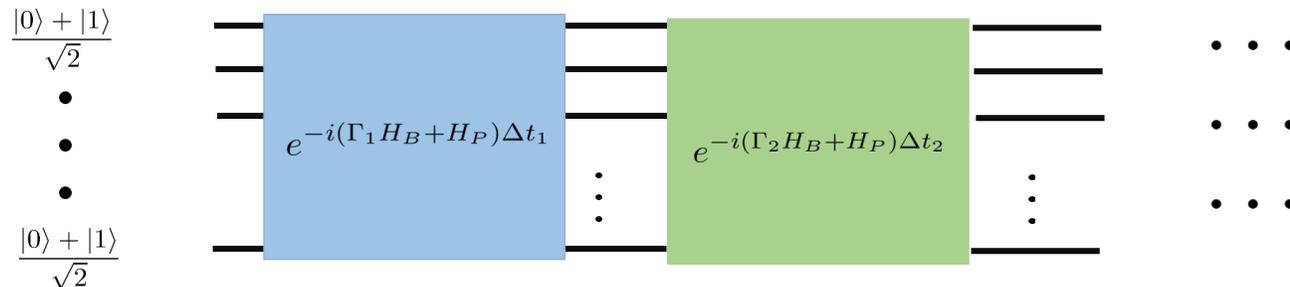
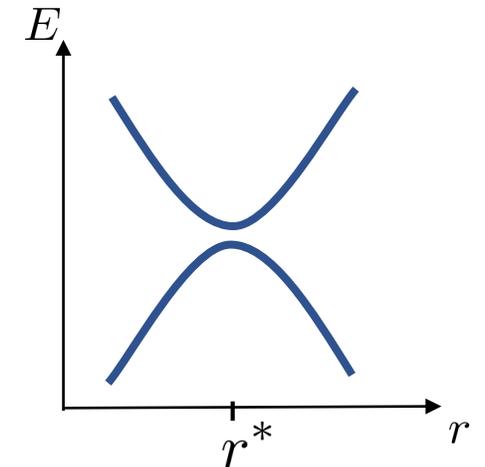
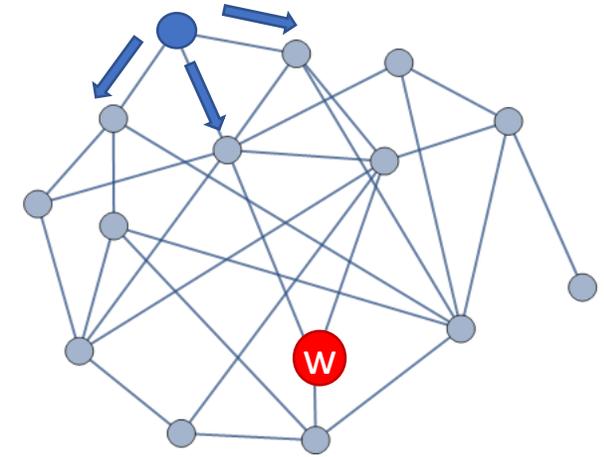
5 stages (Heuristic parameter choices):

$$\frac{\gamma_{i+1}}{\gamma_i} = (1 - \Delta\gamma)$$



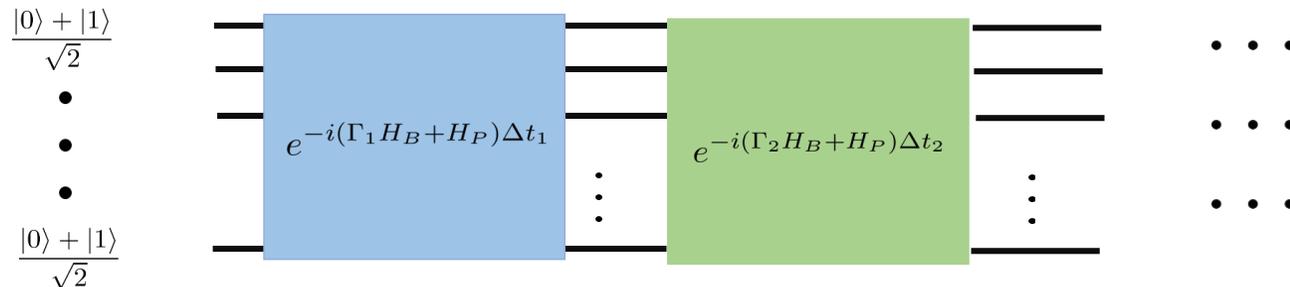
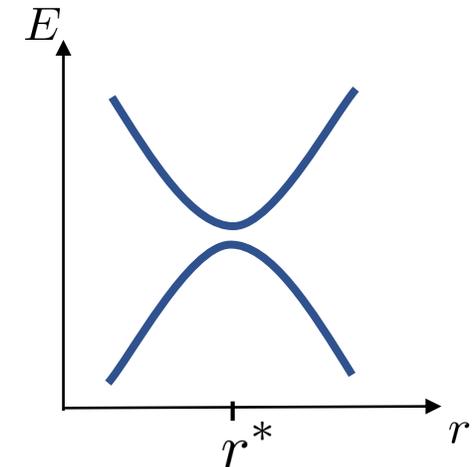
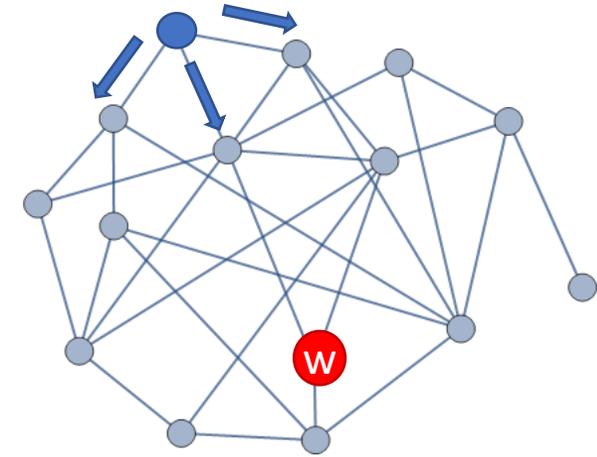
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- CTQW provide simple ways to design **search and optimization** algorithms.
- General results about performance are known for spatial search problems on graphs.
- Identified limitation for **provable** quadratic speed-ups for adiabatic quantum unstructured search.
- A new (**and only?**) **complexity theoretic result** about predicting position of avoided crossing.
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Thank you for your attention!